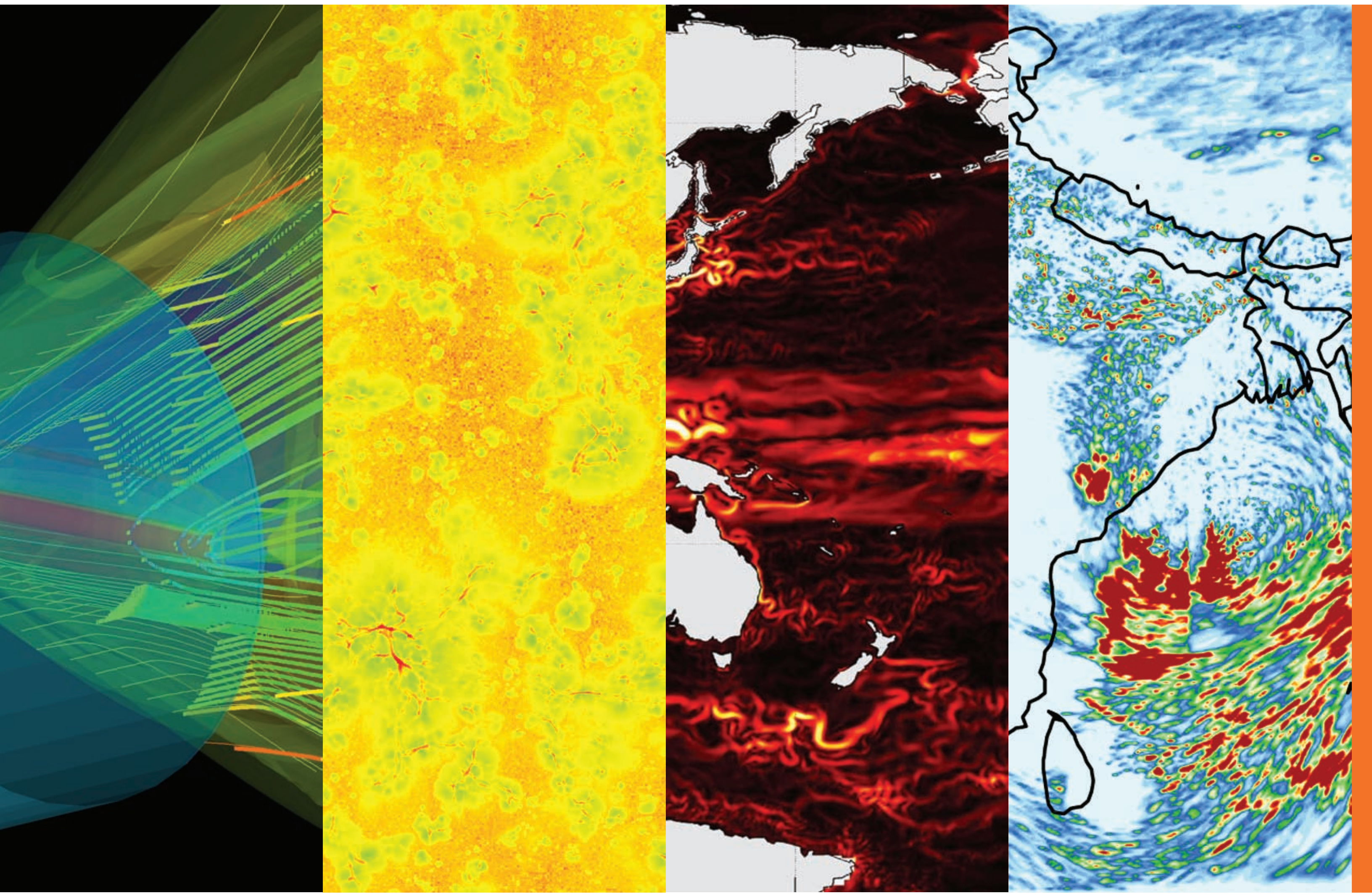

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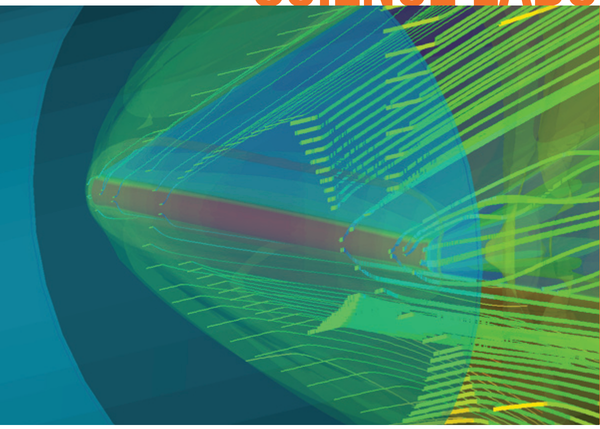
AEROTHERMAL ANALYSIS IN SUPPORT OF MARS SCIENCE LABORATORY HEATSHIELD QUALIFICATION



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◀ Close-up of Figure 1.

Project Description: The Mars Science Laboratory (MSL) is a flagship-class rover mission scheduled for launch in winter 2011. The purpose of this project is to provide computational fluid dynamics (CFD) analysis to support the design, testing, and qualification of the Phenolic Impregnated Carbon Ablator (PICA) heatshield, Super Lightweight Ablator (SLA) backshell, and Acusil-II Parachute Closeout Cone (PCC) thermal protection system (TPS) that will protect the spacecraft from the harsh entry environment at Mars.

This is an applied engineering—as opposed to a research—project. The work consists of aerothermal CFD simulations of the chemically reacting, non-equilibrium hypersonic flowfield around the TPS material samples tested in an arc jet environment. We also analyze the hypersonic flowfield about the MSL spacecraft during Martian entry. Key areas of interest are the turbulent heating and shear stress on the heatshield and the local transient heating rates and flow topologies produced by firing reaction control system (RCS) thrusters on the backshell. The simulations use the Data-Parallel Line Relaxation (DPLR) and the Langley Aerothermodynamic Upwind Relaxation Algorithm (LAURA) codes. DPLR, developed at NASA Ames Research Center by this project's principal investigator and collaborators, was a co-winner of NASA's 2007 Software of the Year Award.

Relevance of Work to NASA: Material testing after the Critical Design Review uncovered a catastrophic failure mode in the baseline heatshield material for MSL. The uncovered failure mode forced the project to change the heatshield TPS material to one with a lower technology readiness level (TRL) because, at the time, there was less than one year to develop, design, and qualify the new concept before launch (the original launch date for MSL was set for October 2009). When MSL management switched the heatshield TPS material, they identified the TPS system as the largest risk item to the entire MSL program. A critical part of the engineering analysis required to reduce this risk is CFD simulations of the arc jet testing performed on the material over the range of expected entry environments, and corresponding analysis of the expected flight environment.

Computational Approach: We test TPS materials using a 60-megawatt test bay at the NASA Ames Arc Jet Complex, as well as smaller facilities at Ames and the Arnold Engineering Development Center. At these energy levels, the supersonic gas that flows over the test articles is highly dissociated and in a state of extreme non-equilibrium. Simulations of this complex flow require state-of-the-art computational tools that can model both the fluid dynamics and the chemical processes involved. We use the DPLR aerothermal CFD code to perform these simulations. Full 3D, non-equilibrium reacting flow Navier-Stokes calculations of the test article in the arc jet flow predict the incident heating, pressure, and shear stress on the model. The simulations are very complex, involving millions of grid points and up to 16 chemically reacting species. We then use these predicted quantities as boundary conditions for another code, which predicts the response of the ablative material. We perform flight simulations using similar physical models in DPLR and LAURA. Similar tools are necessary because the energy content of the flow impacting the flight environment is similar to that encountered in the arc jet.

Results: This project began in October 2007, when MSL management changed the TPS material. Between October 2007 and July 2008, we performed dozens of simulations of both the flight and arc jet environments (Figures 1 and 2). These results successfully demonstrated the adequacy of the PICA heatshield for MSL at the final TPS review in July 2008. Since July, work has continued in support of final developmental tests and in the planning and execution of the qualification test program. Although the mission has been delayed, all elements of the aeroshell TPS were designed, tested, and built in time to support the original launch date.

Role of High-End Computing: The computational power of the Columbia supercomputer at the NASA Advanced Supercomputing (NAS) facility was an enabling capability for this work. The project was extremely schedule-driven given the original, fixed launch date of the spacecraft. It was only with priority access to Columbia that we were able to generate the engineering data to demonstrate that the heatshield would perform.

Future: This project will terminate with the launch of MSL in winter 2011.

Co-Investigators

- Chun Tang, Todd White, Dinesh Prabhu, all of ELORET Corp.
- Karl Edquist, Artem Dyakonov, NASA Langley Research Center
- James Brown, NASA Ames Research Center

Publications

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[4] Prabhu, D., "CFD Analysis Framework for Arc-Heated Flowfields II: Shear Testing in Arc Jets at NASA ARC," submitted to the 41st AIAA Thermophysics Conference, June 2009.

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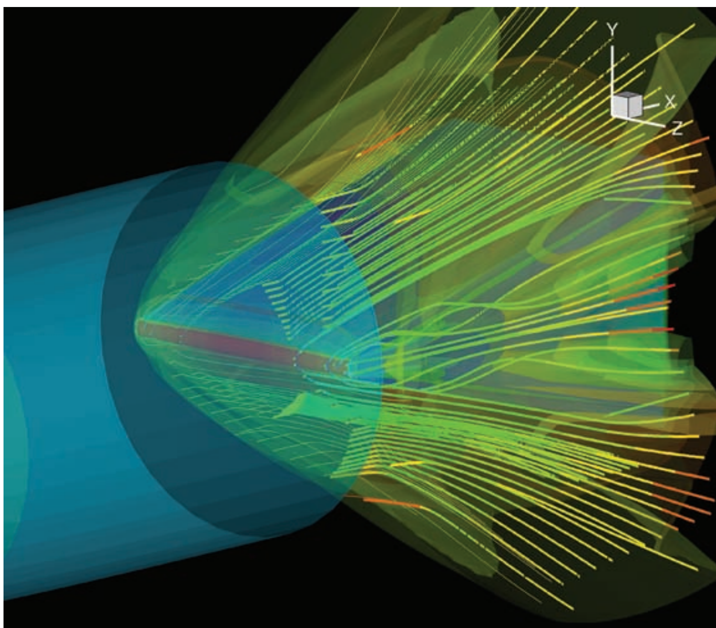


Figure 1: Simulation of a Phenolic Impregnated Carbon Ablator (PICA) wedge sample in shear at NASA Ames Research Center's Interaction Heating Facility. PICA is the heatshield material selected for the Mars Science Laboratory (MSL).

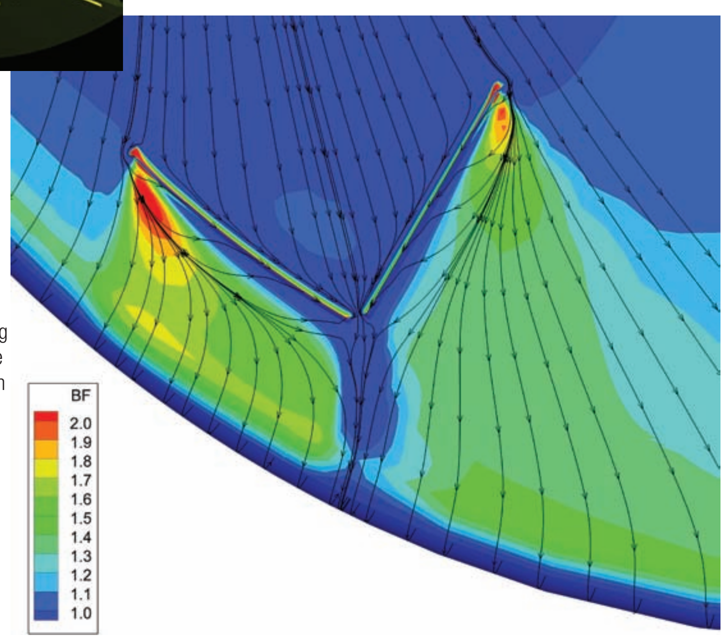
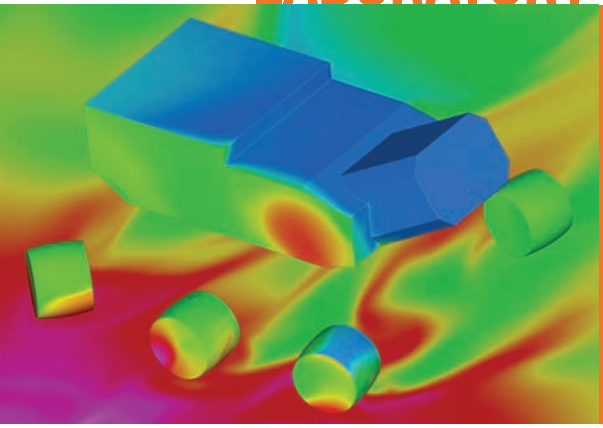


Figure 2: Simulation of an MSL flight heatshield showing augmented heating due to gap-filler protrusion. BF is the bump-factor, defined as the ratio of heating to that which would be encountered with zero protrusion.

CFD SUPPORT FOR MARS SCIENCE LABORATORY ENTRY, DESCENT, AND LANDING



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◄ Close-up of Figure 2.

Project Description: The Mars Science Laboratory (MSL) is a large rover being designed to perform various planetary science tasks on Mars towards the objective of determining whether life existed or could have existed there. The MSL payload and entry system are each at least three times as massive as any previously flown to Mars, but the mission will need to perform a precision landing within an ellipse several times smaller than that of prior missions.

To achieve precision landing capability, the MSL capsule will fly a lifting trajectory with coordinated banked turns to reduce velocity and align with the landing target. A reaction control system (RCS) consisting of eight small rocket engines will steer the vehicle and damp out oscillations. Depending upon vehicle attitude and flow conditions, RCS plumes may interact with external flow to reduce control authority and induce unintended motions. Such phenomena are termed "aero/RCS interactions." Once near landing, the MSL lander-stage will separate from the backshell and parachute to begin descent under power of eight lander-stage rocket engines. Then, an umbilical will lower the rover to the ground in a "skycrane" maneuver during which the Mars lander-stage engine (MLE) plumes impinge on the ground.

The goal of this project is to provide analysis of fluid dynamics phenomena during MSL entry, descent, and landing (EDL). These phenomena include static aerodynamics, aero/RCS interactions, and MLE plume/ground interactions.

We perform computational fluid dynamics (CFD) simulations of MSL EDL elements to attain a better understanding of EDL element behaviors. Of particular interest have been (i) the characterization of MSL and Phoenix capsule (a 2007–08 Mars lander mission) static aerodynamics and aero/RCS interactions (Figure 1); and (ii) MSL MLE plume-induced rover environments (Figure 2). To this end, we run simulations at flight or wind tunnel conditions using the FUN3D, LAURA, and/or OVERFLOW-2 flow solver codes. We compare numerical results against experimental data where available.

Relevance of Work to NASA: This work is part of the MSL EDL analysis being performed at the Atmospheric Flight and Entry Systems Branch of NASA Langley Research Center. Results and lessons learned will help to advance the state of the art in EDL analysis.

Computational Approach: The research uses both unstructured and structured grid methods. Either approach begins with the surface definition of a flight article or wind tunnel model in the form of Initial Graphics Exchange Specification (IGES) files either acquired through the NASA Jet Propulsion Laboratory or constructed from engineering drawings using the commercial code Gridgen. For the unstructured grid approach, we generate grids using the NASA Langley-developed GridTool and VGrid packages and solve flows with the FUN3D solver (also developed at NASA Langley). For the structured approach, we generate grids using Gridgen and the NASA Ames Research Center-developed Chimera Grid Tool package and solve flows with the Langley Aerothermodynamic Upwind Relaxation Algorithm (LAURA) or OVERFLOW-2.

Results: These CFD simulations have made significant contributions to MSL mission design:

- Results from steady-state Phoenix aero/RCS analyses revealed a general lack of robust control authority and possible control reversal about one axis. As a result, the mission team increased the controller deadbands and did not use the RCS during the successful EDL [1].
- Computations showed that early, tangentially firing MSL RCS designs caused large aero/RCS interactions and enhanced aeroheating. These findings led to a configuration change.

- Static aerodynamic coefficients from simulations agreed closely with those measured in the NASA Langley Unitary Plan Wind Tunnel at supersonic Mach numbers.
- MLE plume simulations produced engineering estimates of particle impingement and thermal environments for the MSL rover [2].

Role of High-End Computing: Simulating viscous multispecies flowfields about complex geometries would be daunting without high-end computing. Some simulations were demanding in terms of sheer size, with grids exceeding the 50-million-cell mark, while others required running several combinations of freestream conditions, vehicle orientation, and RCS configuration to yield clear trends. Use of the Columbia supercomputer at the NASA Advanced Supercomputing (NAS) facility made quick turnaround possible, reducing delivery time from weeks or months to hours or days.

Future: Work is continuing on various MSL EDL elements, including subsonic and transonic aero/RCS interaction analysis and MLE plume impingement studies. The overall goal is to provide high-fidelity CFD analyses to help ensure a successful mission.

Co-Investigators

- Pawel Chwalowski, Analytical Mechanics Associates, Inc.
- Pieter Buning, NASA Langley Research Center

Publications

[1] Dyakonov, A., Glass, C., Desai, P., and Van Norman, J., "Analysis of Effectiveness of Phoenix Entry Reaction Control System," AIAA/AAS Astrodynamics Specialist Conference and Exhibit, 2008.

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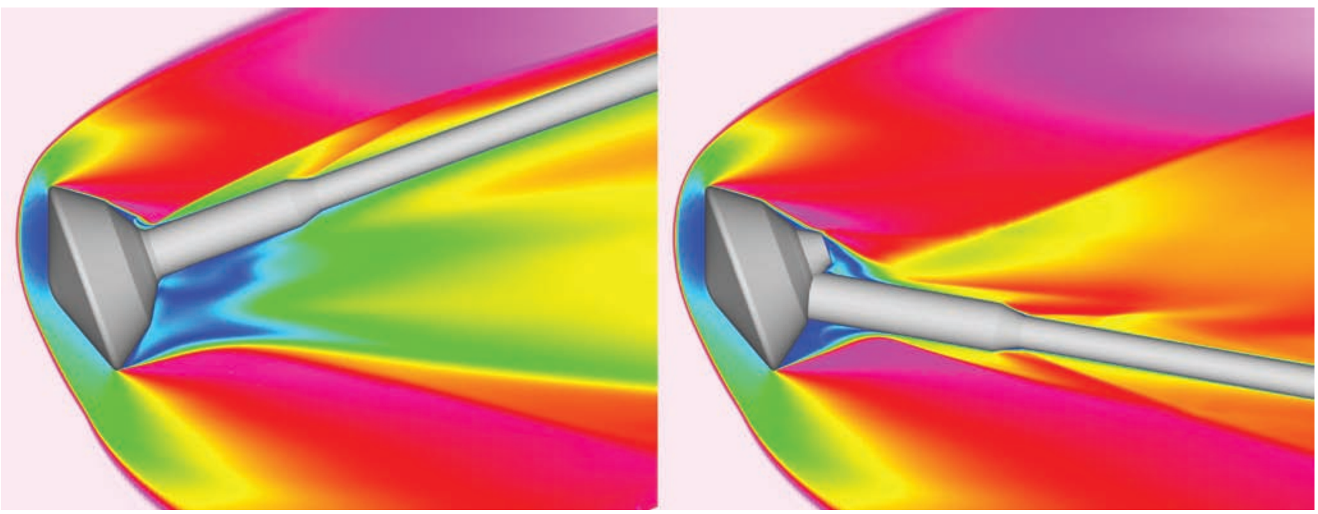


Figure 1: Mach contours surrounding Mars Science Laboratory (MSL) wind tunnel models with axisymmetric (left) and 30° (right) sting configurations at Mach 4.5 and -20° angle of attack.

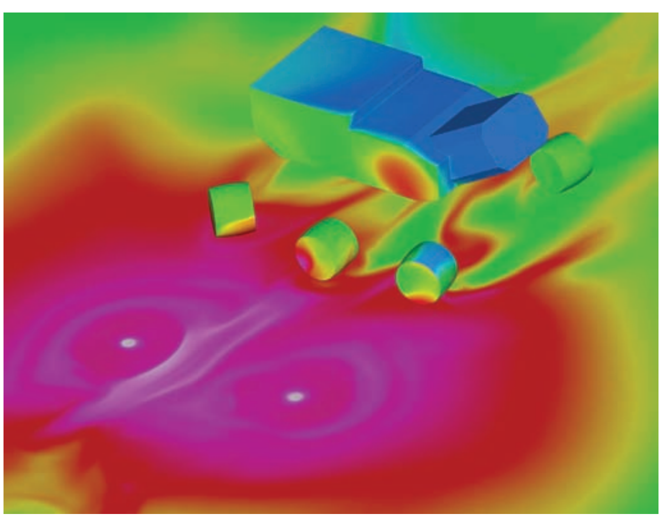
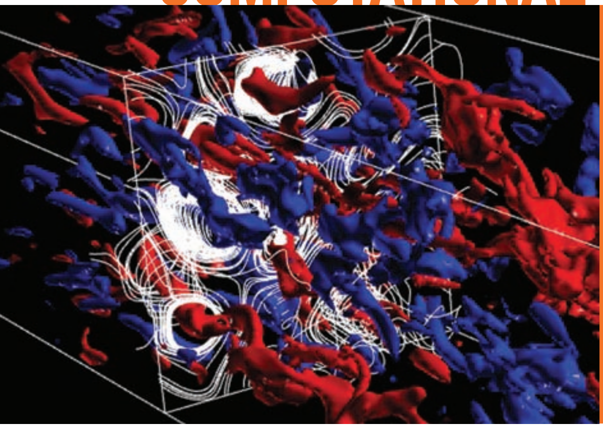


Figure 2: Instantaneous temperature contours surrounding the MSL rover exposed to plumes from the Mars lander-stage engines.

COMPUTATIONAL STUDY OF RELATIVISTIC JETS



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◀ Detail of Figure 1.

Project Description: This project seeks a better understanding of the formation and dynamics of relativistic jets and their emission by supernova remnants, active galactic nuclei, and gamma-ray bursts (GRBs). We are studying how jets form from black holes, how relativistic jets propagate, and how various free-energy sources and their associated heating, acceleration, and plasma transport lead to the excitation of instabilities. We are also investigating ultra-relativistic jets associated with GRBs and their prompt and afterglow emission.

We are using relativistic and general relativistic particle-in-cell (RPIC/GRPIC) and magnetohydrodynamics (MHD) codes with large 3D systems. This research is designed to provide a fundamental understanding of macroscopic relativistic MHD processes, microscopic plasma processes, and observed emissions. Our codes allow us to study the effect of inherent nonlinear processes on plasma dynamics and to compare simulation results with observations and analytical predictions.

Relevance of Work to NASA: Our studies are driven by anticipated new science from present and future NASA missions. The Swift mission has excelled at rapid burst afterglow follow-ups, generating a catalog of GRB redshifts and, in some cases, the properties of their associated supernovae. The Fermi Gamma-Ray Space Telescope investigates the spectra of GRBs over an unprecedented energy span. Our work will help to calculate the emission efficiency and self-consistent spectra expected from GRB relativistic shocks observed by Fermi. Future advanced X-ray telescopes and the Beyond Einstein Program's Black Hole Finder Probe will study other sources of relativistic jets; our work will be crucial to understanding these emissions. Funding from this research comes from NASA's Astrophysics Theory and Fundamental Physics Program.

Computational Approach: Thanks to the NASA Columbia supercomputer's unique structure and support for large 3D systems, we are systematically investigating the dynamics of relativistic jets with three codes:

3D RPIC code: We rewrote an earlier Fortran 77 code using the Message Passing Interface (MPI) and Open Multi-Processing (OpenMP). We have used it for several large simulations, which require terabytes of memory to achieve the necessary resolution and allow the full development of nonlinearities.

3D GRPIC code: The particle motion follows the contravariant form of the Newton-Lorentz equation. The acceleration is a function of the spacetime curvature defined by the metric and the Lorentz force due to the electromagnetic field. The local field is described by the Maxwell field tensor, whose components follow the contravariant general relativistic form of Maxwell's equations. The simulation moves the particles using an adaptive 5th-order Runge-Kutta scheme and calculates the fields and currents self-consistently. We have parallelized this code using MPI.

3D General Relativistic MHD code: "RAISHIN" is a conservative, high-resolution, shock-capturing scheme based on a 3+1 formalism of the General Relativistic MHD equations in a curved spacetime. RAISHIN computes numerical fluxes using the Harten-Lax-van Leer (HLL) approximate Riemann solver scheme. A flux-interpolated, constrained transport (flux-CT) scheme maintains a divergence-free magnetic field. We have vectorized this code and parallelized it using OpenMP.

Results: Several projects are using our simulation models, with the following outcomes:

- *Generation of shock with plowing ambient plasma:* New studies with a larger simulation domain show that continuously injected jets excite the Weibel instability (Figure 1), pile up ambient plasma, and generate a shock.
- *Parallelizing the RAISHIN code with OpenMP:* In test simulations, this code runs 24 times faster using 64 processors.
- *Relativistic MHD simulations of kink instability in force-free helical field:* Using 128 processors, we have run simulations with different magnetic pitch profiles. Preliminary results

show linear growth of kink instability from initial small perturbations and saturation in the non-linear stage (Figure 2). The growth and structure of kink instability is quite different with each pitch profile. Further simulations will study the effect of relativistic jets on kink instability.

- *Magnetic turbulence production by isotropic cosmic-ray ions streaming from supernova remnant shocks:* We have confirmed that the drift of cosmic-ray ions in the upstream plasma generates a turbulent magnetic field. However, field perturbations grow much more slowly than estimated using an MHD approach.
- *Jet formation from a black hole with kinetic processes:* We have developed a GRPIC code to perform simulations in curved space-time near black holes.

Role of High-End Computing: The significant processing power, memory, and data storage available on the NASA Advanced Supercomputing (NAS) facility's Columbia supercomputer meet the demands of our 3D codes. For example, we completed a recent RPIC simulation in less than 10 days using 320 processors. NASA's High-End Computing personnel are helping us to optimize the MPI code, maintaining temporary disk storage for diagnostics, and supporting 3D visualizations.

Future: We will continue to perform studies with larger simulation domains, which are essential to understanding the physics involved.

Co-Investigators

- Yosuke Mizuno, University of Alabama in Huntsville
- Jacek Niemiec, Polish Academy of Sciences
- Michael Watson, Fisk University

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[1] Hardee, P., Mizuno, Y., and Nishikawa, K.-I., "GRMHD/RMHD Simulations and Stability of Magnetized Spine-Sheath Relativistic Jets," *Astrophysics & Space Science*, vol. 311, pp. 281–286, 2007.

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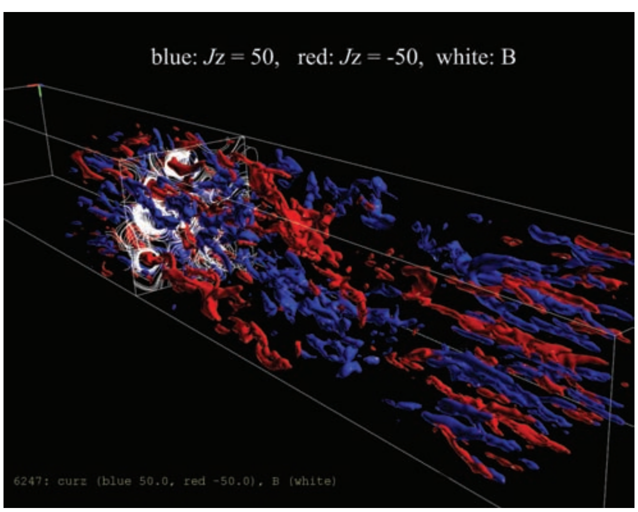


Figure 1: A snapshot viewed from the front of a relativistic jet at t = $59.8/\omega_{pe}$ showing an isosurface of the z-component of the current density (±Jz) and the magnetic field lines (white) at the linear stage.

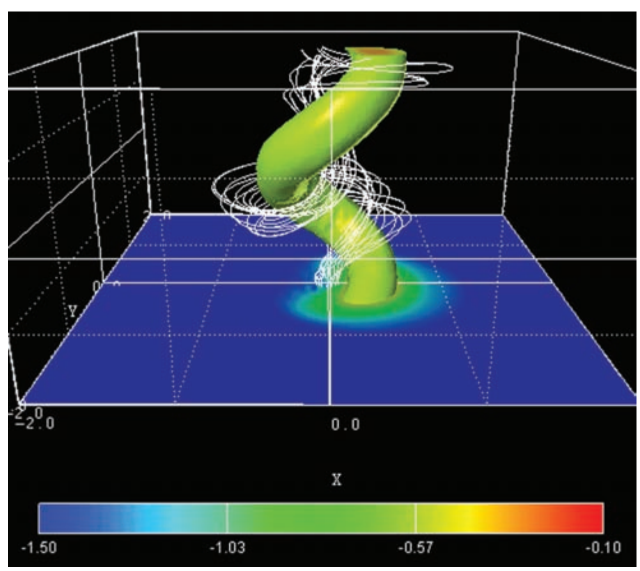
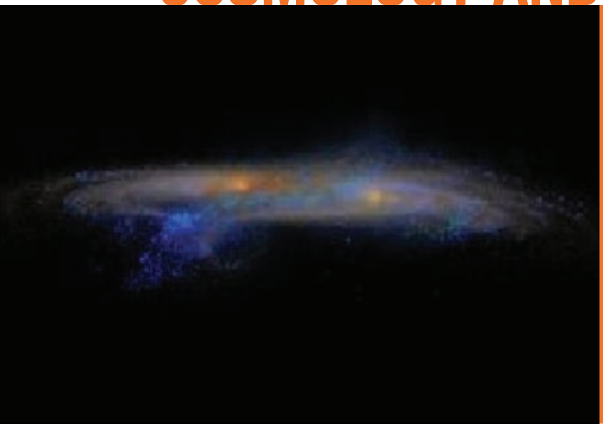


Figure 2: A snapshot of 3D isovolume density with magnetic field lines (white) at the non-linear stage of current-driven kink instability.

COSMOLOGY AND GALAXY FORMATION



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◀ **Figure 1:** A side-view snapshot from a simulated merger of two Sbc spiral galaxies, showing the first pass of the galaxies 0.59 Gigayears (590 million years) into the simulation.

Project Description: According to the now-standard Lambda Cold Dark Matter (ΛCDM) "double dark" theory, almost all of the universe is invisible dark matter and dark energy. This theory successfully predicted the distribution of temperature anisotropies in the cosmic background radiation measured by NASA's Wilkinson Microwave Anisotropy Probe (WMAP), and the distribution of nearby and high-redshift (distant) galaxies. Our project attempts to understand the structure and distribution of dark matter halos in ΛCDM and the formation and evolution of galaxies within the cosmic web. This requires modeling the complex hydrodynamics at cosmological and smaller scales (including the formation of stars and supermassive black holes) and their effects in heating the surrounding gas and providing the heavy elements from which planets form.

We are conducting high-resolution hydrodynamic simulations of mergers of gas-rich disk galaxies, which may form many of the fast-rotating elliptical galaxies. We have also created an analytical model that correctly predicts the properties of such elliptical galaxies, allowing us to interpolate between simulated cases and extrapolate beyond them. This work lets us calculate the entire evolving population of early-type galaxies. We are also doing hydrodynamic simulations of cold gas inflows and multiple mergers at high redshifts $z \sim 2$, which may form the ~25% of elliptical galaxies classified as slow rotators. Finally, we are running large dissipationless simulations, including a constrained realization of our local region of the universe and our "Bolshoi" simulation of a volume approximately 1 billion light years (1 Gigalightyear) on a side. The latter uses the new 5th-year cosmological parameters from WMAP and has mass and force resolution an order of magnitude better than the European Virgo Consortium's Millennium Run.

Relevance of Work to NASA: A key challenge in astronomy is to explain how the structures in today's universe formed within the ΛCDM framework and to test these new theories against observational evidence, e.g., from NASA's Hubble, Chandra, Spitzer, and Fermi space telescopes. The theories we are developing and simulating help to predict and interpret observations, and to design future missions such as the James Webb Space Telescope and Joint Dark Energy Mission. We are providing the main theoretical support for the Deep Extragalactic Evolutionary Probe (DEEP) and All-wavelength Extended Groth strip International Survey (AEGIS), which incorporate extensive data from NASA's space observatories. Primary funding for this research comes from NASA's Astrophysics Theory and Fundamental Physics Program, with additional funding from Spitzer and Hubble theory grants.

Computational Approach: Our large dark matter cosmological simulations use the dissipationless Adaptive Refinement Tree (ART) code. For hydrodynamic simulations, we use both ART-Hydro and the smooth-particle hydrodynamics code known as GADGET. Our binary galaxy merger simulations use GADGET. Our cosmological merger simulations start from a large ART-Hydro simulation; from this we map regions into GADGET, splitting particles and using other techniques to achieve an order of magnitude higher resolution. In these simulations, we use our Sunrise code to predict the effects of cosmological dust, which absorbs about 9/10 of the light of the bright new stars produced in galaxy mergers and re-radiates it at longer (infrared) wavelengths.

Results: We have characterized star formation in galaxies formed from binary mergers involving a variety of mass ratios [1]; characterized the morphologies of the resulting early-type galaxies including the effects of dust using our Sunrise code [2] (Figures 1, 2); and compared merger predictions with AEGIS data [3]. We developed an analytic model that correctly predicts the properties of elliptical galaxies formed from binary mergers of disk galaxies [4], and found that mergers of gas-rich disk galaxies with properties given by recent semi-analytic models lead to formation of elliptical galaxies with the observed size-mass relations from high redshift $z \sim 3$ to low redshift $z < 0.5$ [5]. We have simulated multiple mergers of galaxies at redshifts $z \sim 2$, including higher-resolution resimulations of regions identified in a large hydrodynamic simulation. In these simulations, the resulting galaxies resemble the observed slowly rotating elliptical galaxies that are not produced by binary mergers [6].

Role of High-End Computing: The Columbia and Pleiades supercomputers at the NASA Advanced Supercomputing (NAS) facility have been extremely helpful in running dissipationless and hydrodynamic simulations of large-scale structure evolution and hydrodynamic simulations of galaxy mergers, including development and use of our Sunrise code. In particular, our Bolshoi Gigalightyear simulation harnesses the power of Pleiades. Collaboration with the NAS Visualization Group has been crucial in visualizing and interpreting the results of these simulations. These visualizations are helping astronomers and the wider public (e.g., planetarium visitors) to understand the evolving cosmos.

Future: The Bolshoi simulation will become the basis for a higher-resolution merger tree to enable models of unprecedented detail, which will capture earlier stages in galaxy formation and follow the dark matter substructure to small scales where galaxies merge. We intend to make public not only the analyzed results but also the entire merger tree, so that groups around the world can base models on it.

Co-Investigators

- Anatoly Klypin, New Mexico State University

Publications

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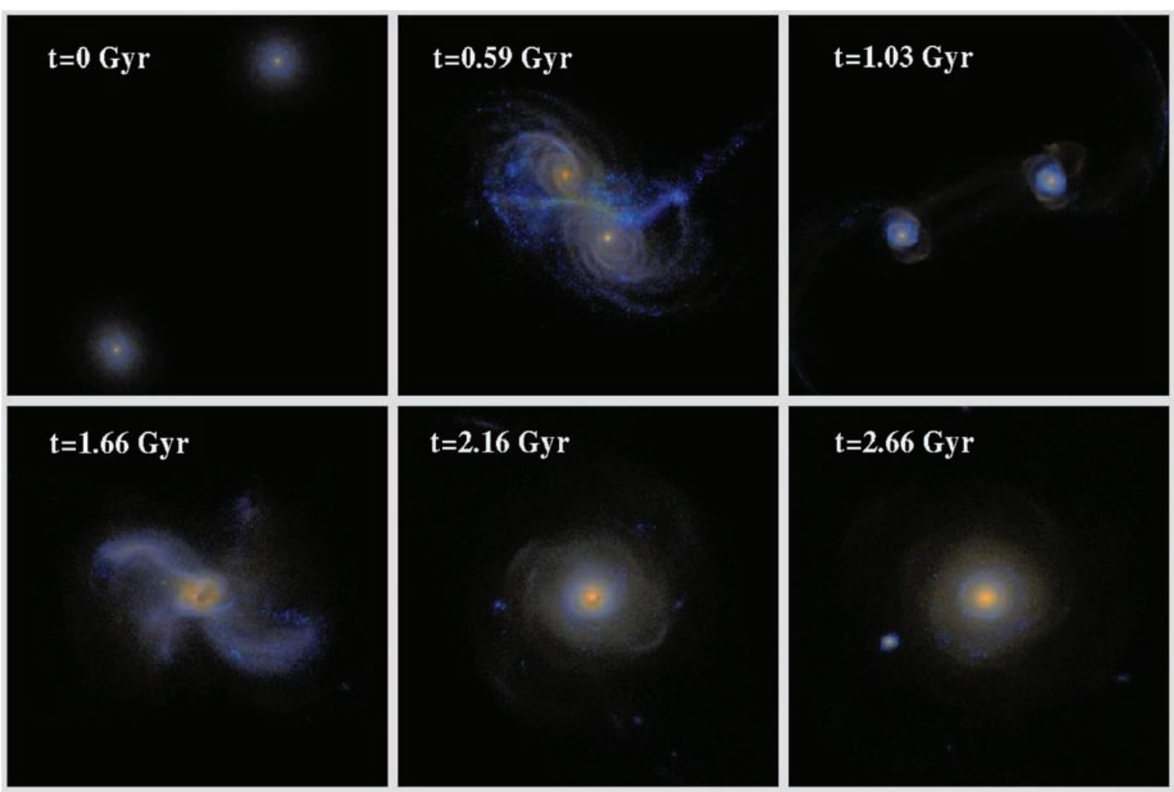

Figure 2: These front-view, u-r-z composite color images with dust extinction come from a simulated merger of two Sbc spiral galaxies over 2.66 Gigayears (Gyr). Top row: initial pre-merger galaxies, the first pass, and subsequent maximal separation. The first and third images are 200 kiloparsecs (kpc) across; the second is 100 kpc. Bottom row: 100-kpc views of the merger and post-merger 0.5 Gyr and 1 Gyr later. Star-forming regions in the initial discs, tidal tails, and outer regions of the remnant appear blue; dust-enshrouded star-forming nuclei appear red [2].

COUPLED OCEAN AND ATMOSPHERE DATA ASSIMILATION SYSTEMS FOR CLIMATE STUDIES

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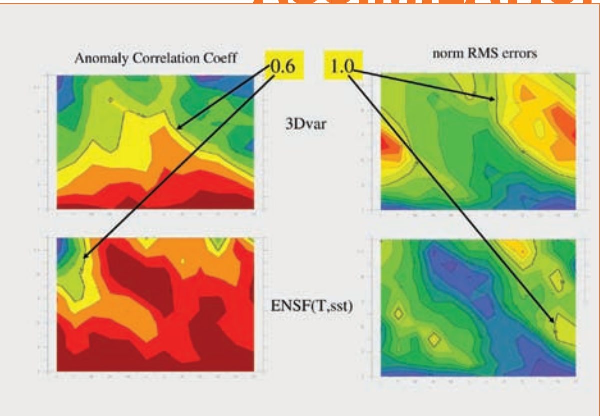

Figure 1: The El Niño-Southern Oscillation forecast skills, including sea-surface temperature anomaly correlation coefficients (left) and normalized Root-Mean-Square errors over the East Pacific area (right). The coupled model ensemble is initialized from the coupled data assimilation products for the last quarter of the 20th century using both atmospheric and oceanic observations.

Project Description: Climate changes occur in a coupled Earth system that includes the atmosphere, ocean, land, and sea-ice components. Due to incomplete understanding of the dynamical and physical processes, modeling is always uncertain, and generated simulations drift away from real-world scenarios. Climate modeling includes predicting future changes as well as assessing historical variations. The necessary estimates of climate states and initial conditions come from data assimilation—blending observational data with coupled models. Assimilation requires massive computational resources.

With computational support from the NASA Advanced Supercomputing (NAS) Facility, the National Oceanic and Atmospheric Administration (NOAA) Geophysical Fluid Dynamics Laboratory (GFDL) has developed a coupled data assimilation (CDA) system consisting of an ensemble filter applied to a fully coupled global climate model (CGCM). Within the coupled framework, the assimilation provides a self-consistent, temporally continuous estimate of the model state and its uncertainty. This estimate takes the form of discrete ensemble members that can be used to directly initialize probabilistic climate forecasts with minimal initial coupling shocks. GFDL's CDA system serves as an estimator of historical climate variations and a predictor of future climate changes. Compared to traditional methods, the CDA system has several advantages:

- Directly solves a temporally evolving, joint-distribution function of climate states under observational data constraints.
- Uses a multi-variate analysis scheme maintaining physical balances among state variables and coupled components.
- Has minimal initial shocks for numerical climate forecasts.

Relevance of Work to NASA: Climate studies and predicting future climate changes are one of the common missions between NOAA and NASA. Efforts such as GFDL's CDA system support the research objectives of NASA's Earth Science Division, particularly the Climate Variability and Change Focus Area objective to "Understand the role of oceans, atmosphere, and ice in the climate system and improve predictive capability for its future evolution."

Computational Approach: To meet the need for accurately assessing historical climate variations and predicting future climate changes, we have developed an ensemble CDA system. Our implementation views the evolution of climate states as a continuous, stochastic, and dynamic process. The filtering assimilation combines an observational probability density function (PDF) with a prior PDF derived from the CGCM to produce an analyzed PDF. Using a super-parallelization configuration, the coupled assimilation is a continuous data-incorporation process that includes atmospheric and oceanic data assimilation components (Figure 3).

Results: Climate Detection Experiments using GFDL's CDA system on NASA's High-End Computing (HEC) systems indicate that the assimilation with the greenhouse gas and natural aerosol radiative forcing at fixed pre-industrial (1860) levels produces a consistent multidecadal warming trend in almost all oceans with its own interannual variability (Figure 2). For oceans that have reasonable observation coverage (e.g., the Pacific and North Atlantic Oceans), the ocean data assimilation process retrieves the trend and the variability quite well, with faster spin-up times and reduced uncertainty.

We have initialized climate estimates and forecasts from observed atmospheric and oceanic data (Figure 1). Hindcast statistics show that this ensemble climate state estimate and prediction system improved ENSO forecast skills dramatically. This improvement happens mainly because the self-consistent ensemble initial conditions from this coupled assimilation system keep all components of the coupled model in a physically balanced state, which helps model dynamics project initial signals onto a seasonal-interannual time-scale.

Role of High-End Computing: Our flagship climate models, CM2.0 and CM2.1, are based on the GFDL Flexible Modeling System, a software environment for developing new physics and new algorithms concurrently, and for expressing them on a variety of HEC architectures, spanning distributed and shared memory, as well as vector architectures. Results from these models served as inputs to the International Panel on Climate Change Fourth Assessment Report. NASA HEC resources at the NAS facility have enabled us to run a significant number of trials and tests of these models. Our efforts have included testing and evaluating the CDA system's performance and scaling. Access to NAS' Columbia supercomputer has been essential for meeting the demands of huge computational resources for climate estimation and prediction using our CDA system.

Future: In the future, we will reorient the CDA system to focus on multi-decadal-scale climate predictions that require assimilating a greater number of observations coherently into a more advanced coupled model—including higher resolutions and more comprehensive physical processes. This undertaking will require a much more powerful computational resource.

Co-Investigators

- Anthony Rosati, Shaoqing Zhang, NOAA Geophysical Dynamics Fluid Laboratory

Publications

[1] Zhang, S., Rosati, A., Harrison, M.J., Gudge, R., and Stern, W., "GFDL's Coupled Ensemble Data Assimilation System, 1980–2006 Oceanic Reanalysis and Its Impact on ENSO Forecasts," Third World Climate Research Programme International Conference on Reanalysis, Tokyo, Japan, Jan. 27–Feb. 2, 2008, 2008.

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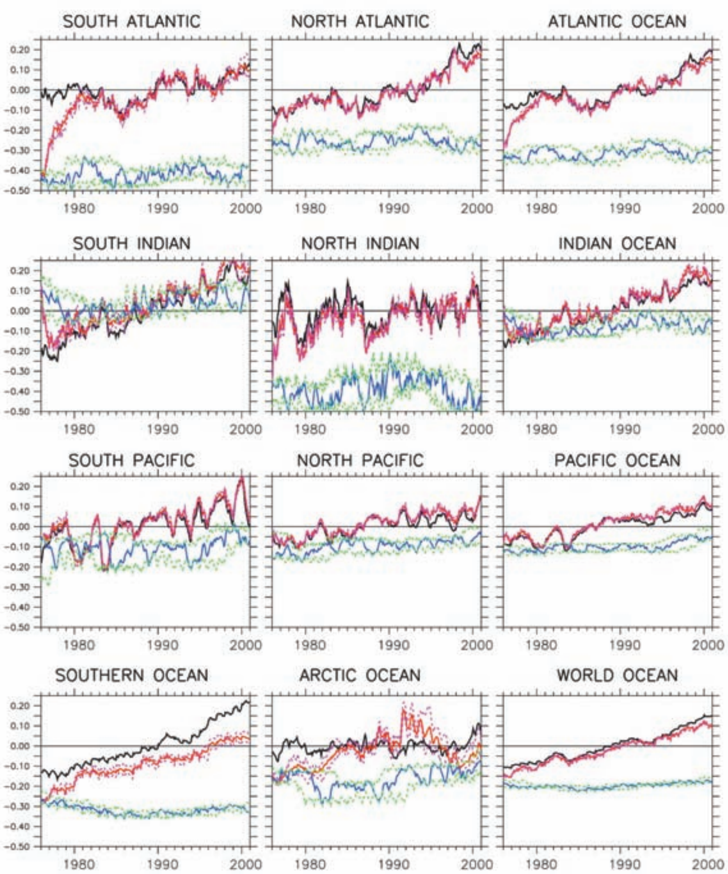


Figure 2: Time series showing the anomalies of the top-500-meter ocean heat content (averaged temperature) in different oceans for the observed "truth" (in black; based on time-varying radiative forcings of greenhouse gases and natural aerosols); the coupled data assimilation (CDA) (red); and the control (blue). The green/pink dashed lines plot the upper/lower bounds of the control vs. CDA spread, which are estimated by the model/assimilation ensemble. All anomalies are computed using observed climatology.

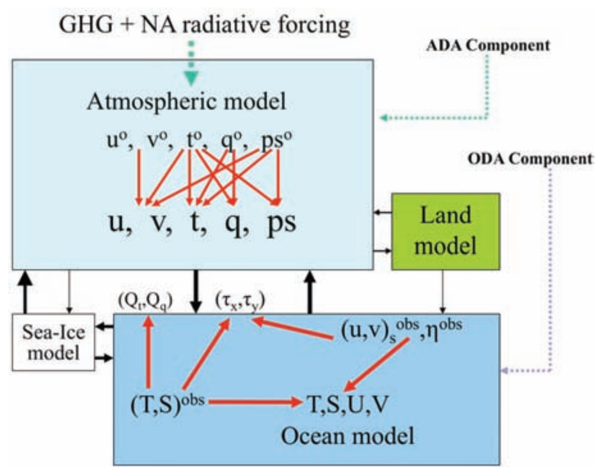
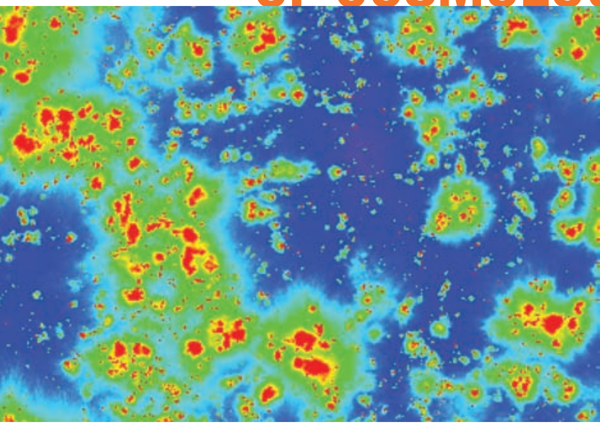


Figure 3: A Geophysical Fluid Dynamics Laboratory coupled climate model exchanges fluxes between model components (atmosphere, land, ocean, and sea-ice models); constraints of atmospheric temperature and wind; and oceanic temperature (T), salinity (S), and currents (U,V) from atmospheric and oceanic data assimilations (ADA/ODA). To isolate 20th century anthropogenic effects, the atmospheric component models the effects of radiative forcing due to both contemporaneous (time-varying) and pre-industrial (fixed 1860) levels of greenhouse gases (GHG) and natural aerosols (NA).

DETAILED SIGNATURES OF COSMOLOGICAL REIONIZATION



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◀ Close-up of Figure 1.

Project Description: The primary goals of this project are to understand the complex cosmological reionization process using detailed radiative transfer hydrodynamics simulations and to provide concrete, detailed observables to confront with current and upcoming observations of the high-redshift universe ($z > 6$). Sometimes called "cosmic dawn," the reionization period began roughly 300 million years after the Big Bang. As the earliest stars appeared, they generated enough ultraviolet light to turn hydrogen atoms back into protons and electrons. These regions of reionization continually expand until they overlap, marking the end of cosmological reionization.

Our cosmological reionization simulations are among the most advanced of their kind, featuring a simulation box on the order of 100 megaparsecs (Mpc) in size, a very high mass resolution (around 1 million solar masses), accurate 3D radiative transfer (using a ray-tracing method), and 3D hydrodynamics. They resolve ionizing, photon-producing galaxies using at least 26 billion particles. The computations couple a total variation diminishing (TVD) hydrocode, to follow hydrodynamics of the cosmic gas, and a 3D ray-tracing code, to follow the propagation of cosmological reionization fronts.

Such simulations serve two primary purposes: First, they provide the most accurate characterization of the reionization process, which allows direct comparison to a wide range of observations spanning the entire electromagnetic spectrum. These include 21-centimeter observations of the neutral hydrogen evolution, as well as forthcoming observations of the first galaxies by the James Webb Space Telescope (JWST), and of intervening free-electron polarization of the cosmic microwave background (CMB) by the European Planck mission. Second, we can use our simulations to calibrate faster, semi-numerical methods, which are necessary for exploring the vast parameter space that reflects our limited knowledge of the high-redshift universe.

Relevance of Work to NASA: These simulations will provide a quantitative framework for interpreting observations by NASA and others, including the Wilkinson Microwave Anisotropy Probe (WMAP), JWST, and Planck. Our simulations will help explore the last, high-redshift ($z > 6$) frontier of the universe, where several cosmic landmarks occur, including: the formation of the first stars, the appearance of the first galaxies; and the first enrichment of the pristine cosmic gas by the metals synthesized in the stars, which will shape the subsequent evolution of galaxies and the intergalactic medium. Our research program supports NASA's mission to "pioneer the future in space exploration, scientific discovery, and aeronautics research," and directly advances the research objectives of the Astrophysics theme "Origin and Evolution of Cosmic Structure" in the *Science Plan for NASA's Science Mission Directorate 2007–2016*. NASA funding for our project comes from the Astrophysics Theory and Fundamental Physics Program.

Computational Approach: RADHYDRO is a hybrid code that combines a very-high-resolution N-body code, a shock-capturing TVD hydrodynamics code, and a ray-tracing radiative transfer code. It allows us to simultaneously compute the formation of low-mass, high-redshift galaxies and the evolution of the intergalactic medium and the fluctuating ionizing radiation background. RADHYDRO is fully parallelized using OpenMP.

Results: We carried out the world's largest 3D radiative transfer hydrodynamics simulations of cosmological reionization. One simulation, run on the NASA Advanced Supercomputing (NAS) facility's Columbia supercomputer, tracked nearly 29 billion dark matter particles on a computational mesh with more than 1.5 trillion cells. We also showed that an inhomogeneous reionization process imprints important signatures on the intergalactic medium, even in the lower-redshift regions already accessible to observations [1] (Figures 1 and 2).

From our results, the NAS visualization team has produced visualizations that have received broad exposure in venues such as the Museo di Storia Naturale (Natural History Museum), Trieste, Italy, and SC08: The International Conference for High-Performance Computing, Networking, Storage, and Analysis, Austin, Texas.

Role of High-End Computing: The RADHYDRO code requires a large symmetric multiprocessing (SMP) machine; the Columbia supercomputer at NAS is the best available platform for this application. The NAS visualization team led by Chris Henze provided an extremely valuable service in helping us visualize the complex data produced by our simulations to yield a form with high public outreach value, in addition to the intrinsic scientific value.

Future: We will expand our usage of the HEC resources continuously and expect to make still larger and better simulations in the next several years, in anticipation of and preparation for the launch of major missions, including Planck and JWST.

Publications

[1] Trac, H., Cen, R., Loeb, A., "Imprint of Inhomogeneous Hydrogen Reionization on the Temperature Distribution of the Intergalactic Medium," *The Astrophysical Journal Letters,* Volume 689, Issue 2, pp. L81–L84, 2008.

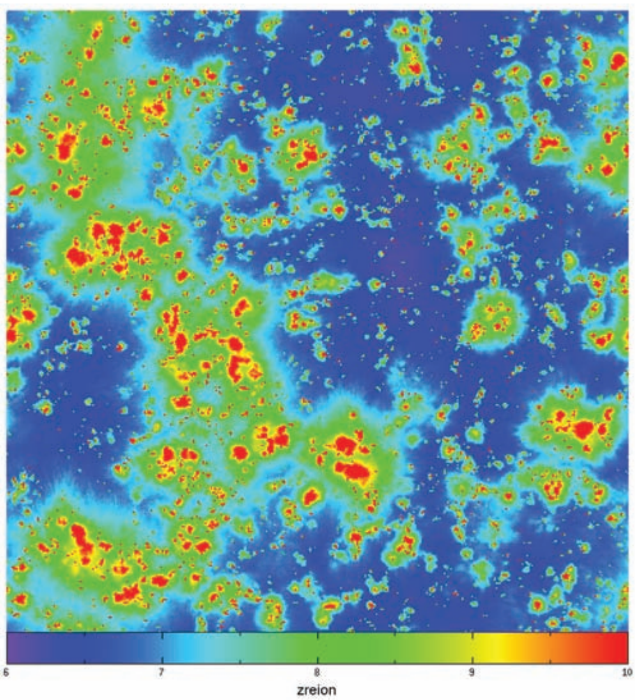

Figure 1: This visualization shows a 100-megaparsec-squared (100 Mpc)^2 slice with a thickness of two hydrodynamics cells (130 kiloparsecs) from the late reionization model of cosmological formation. Coloring traces the redshifts of reionization in the individual cells.

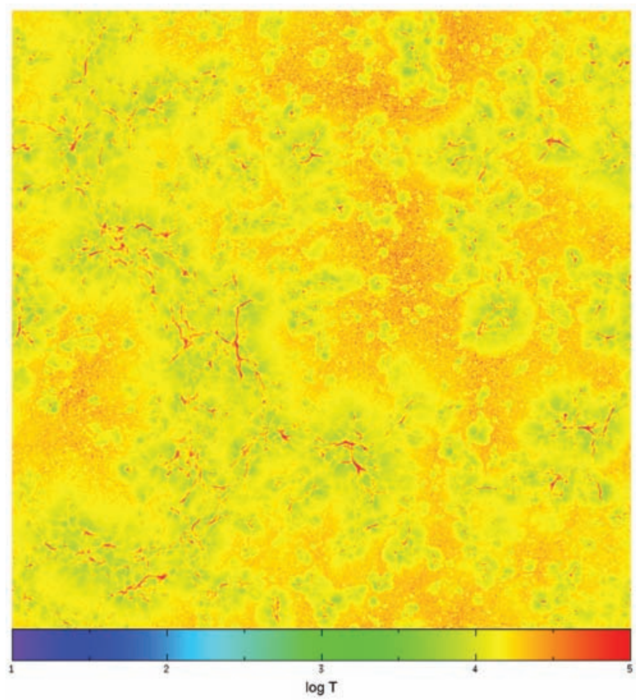

Figure 2: This image is a visualization of the same simulation domain; colors indicate the temperature at the end of reionization.

GEOS-5/MODERN ERA RETROSPECTIVE-ANALYSIS FOR RESEARCH AND APPLICATIONS (MERRA)

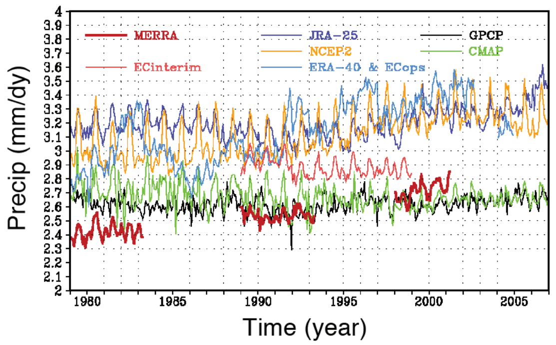

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Figure 1: Global monthly mean precipitation (millimeters/day) from the three MERRA streams (as of November 13, 2008) compared with observations from the Global Precipitation Climatology Project (GPCP) and the NOAA Climate Prediction Center (CPC) Merged Analysis of Precipitation (CMAP). Also shown are other centers' previous (NCEP and ERA-40) and ongoing (ECInterim and JRA-25) reanalyses. MERRA, focused on the hydrological cycle, is closer to the observations. All reanalyses are sensitive to changes in the observing system.

Project Description: Retrospective analyses (or reanalyses) synthesize temporally and spatially irregular observations from the historical observational databases to provide a gridded record of essential climate variables. The model-data synthesis (analysis) uses a "frozen" data assimilation system (DAS) to provide a consistent view, in space and time, of observations from different sources and of different types. The synthesis also provides a view of unobserved variables consistent with those observed. The Modern Era Retrospective-analysis for Research and Applications (MERRA) is producing an atmospheric retrospective-analysis of the satellite era (1979 to present) in order to improve upon previous reanalyses of the hydrological cycle and minimize the influence of observing system changes on the representation of climate variability and trends.

The DAS used for MERRA consists of the Goddard Earth Observing System, Version 5 (GEOS-5) atmospheric model coupled to the Grid-point Statistical Interpolation (GSI) analysis scheme being developed by the National Centers for Environmental Prediction's Environmental Modeling Center (NCEP/EMC) and NASA's Global Modeling and Assimilation Office. Unlike earlier reanalyses, MERRA uses the GSI's online satellite radiance bias correction and includes updated cross-satellite calibrations for the Special Sensor Microwave/Imager (SSM/I) and Microwave Sounding Unit (MSU) to reduce artificial variability associated with the change of satellite platforms. In addition to satellite radiances, MERRA assimilates several remotely sensed retrieved datasets (e.g., SSM/I surface winds and cloud track winds) and conventional observations from radiosonde, dropsonde, aircraft, and surface pressure instruments. Figure 2 depicts the observing system at various points over recent decades.

Relevance of Work to NASA: MERRA supports NASA's climate science by placing current research satellite observations in a climate context. It provides a gridded historical record of meteorology for performing climate diagnostics, initializing and validating climate predictions, and undertaking studies with atmospheric constituent transport and ocean and land surface models. By focusing on an improved representation of the water cycle, MERRA also supports NASA's programs to characterize and predict Earth's energy and water cycles. GEOS-5 and MERRA are supported by the NASA Modeling, Analysis, and Prediction (MAP) Program. Additional MERRA support comes from NASA's Research, Education, Applications Solutions Network (REASoN).

Computational Approach: GEOS-5 uses finite-volume dynamics on a spherical grid. The MERRA configuration has a 2/3-degree longitude by 1/2-degree latitude grid with 72 vertical levels to 0.01 hectopascals (hPa), with assimilation analyses every 6 hours. The GSI uses a 3D variational approach to solve the least-squares fit of GEOS-5 analysis states to the model (background) states and to the available satellite and *in situ* data. Recursive filters are the basic building blocks used to create background error covariance structures.

Results: For MERRA, the GEOS-5 DAS has undergone tuning, with a focus on the hydrological cycle rather than weather prediction skill as for other systems used for reanalysis (Figure 1). We validated the MERRA system by comparing analyses for each season in 2004 and for January 2006 against independent data and other reanalyses. The validation activity was comprehensive and included investigation of climate phenomena such as monsoons, low-level jets across the U.S., the diurnal cycle of precipitation, radiative forcing diagnostics, precipitation distributions, and many other aspects [3]. We also conducted limited sensitivity experiments to gauge the impact of satellite bias estimates and new observing systems such as SSM/I. These experiments showed that we should expect a 10% increase in tropical precipitation in MERRA solely from the introduction of SSM/I [4]. In May 2008, after validation and external review, MERRA began delivering product collections to the Goddard Earth Science Data

Information and Services Center (GES-DISC - http://disc.sci.gsfc.nasa.gov/MDISC/), where the data are available on-line.

Role of High-End Computing: To process the 30-year observational record (in three 10-year streams), MERRA requires continuous access to 432 processors of the Discover system at the NASA Center for Computational Sciences (NCCS) over 18 months. MERRA will generate about 70 terabytes of data products and a similar volume of intermediate archive data.

Future: MERRA will complete the 30-year reanalysis to 2008 in about August 2009. We are conducting observing system sensitivity experiments by withholding the Earth Observing System (EOS) data streams to evaluate the impact of these research data on the inferred climate. Other sensitivity experiments will help to estimate uncertainty due to model and assimilation configurations (e.g., resolution, covariance models, improved estimates of emissivity for radiative transfer calculations) and datasets (e.g., using only data types available prior to the introduction of SSM/I in August 1987).

Co-Investigators

- Max Suarez, Ron Gelaro, Julio Bacmeister, Emily Hui-Chun Liu, Ricardo Todling, Michael Bosilovich, Siegfried Schubert, Gi-Kong Kim, Junye Chen, all of NASA Goddard Space Flight Center

Publications

[1] Rienecker, M.M., et al., "The GEOS-5 Data Assimilation System – Documentation of Versions 5.0.1, 5.1.0 and 5.2.0," *NASA GSFC Technical Report Series on Global Modeling and Data Assimilation*, NASA/TM-2008-104606, Vol. 27, 101 pp. (http://gmao.gsfc.nasa.gov/pubs/docs/GEOS5_104606-Vol27.pdf), 2008.

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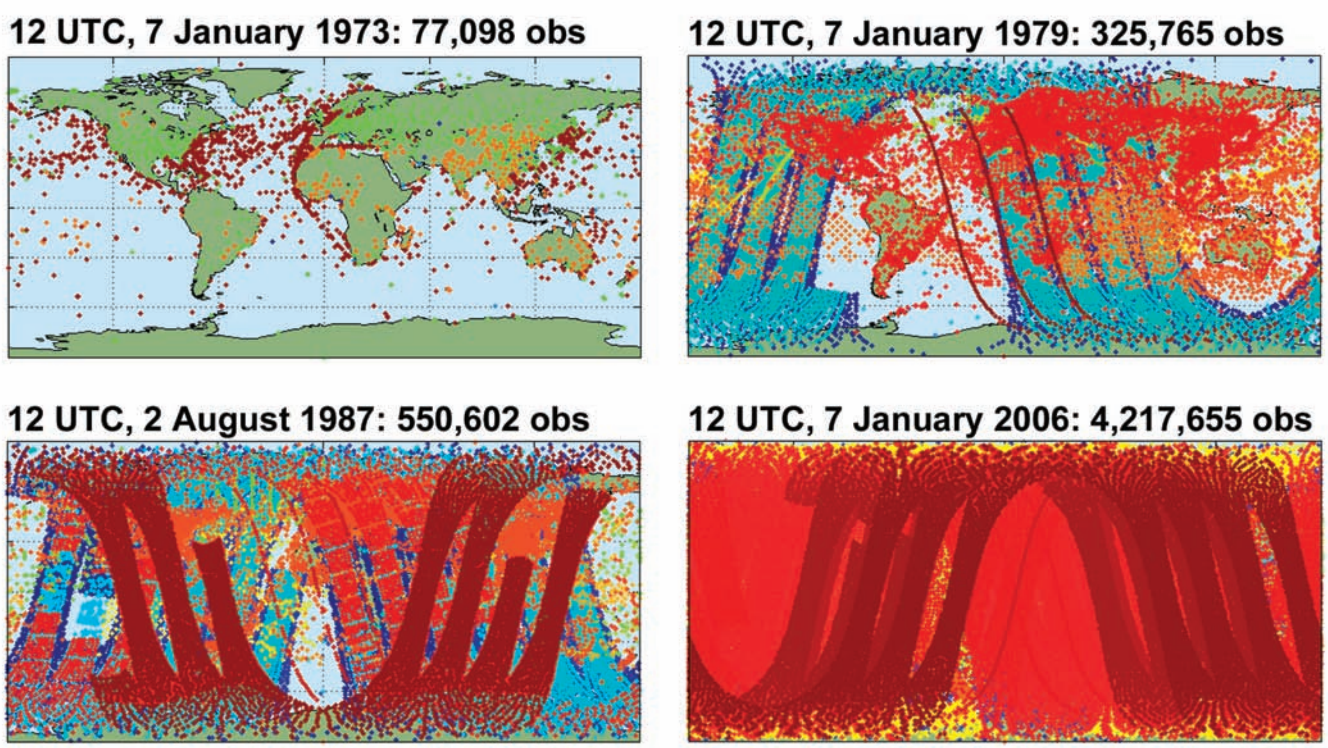
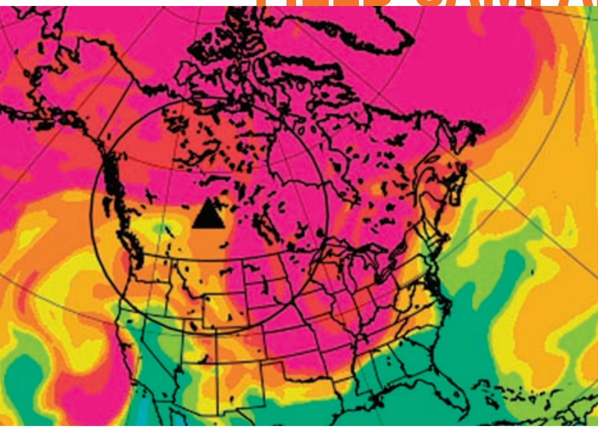


Figure 2: The number of atmospheric observations to be assimilated has increased dramatically over the last few decades. The panels show the evolution of observing systems from 1973 (pre-satellite) to 1979 (TIROS Operational Vertical Sounder [TOVS]) to 1987 (add Special Sensor Microwave Imager [SSMI]) to 2006 (add Atmospheric Infrared Sounder [AIRS]). Each color represents a different observing system, and the titles list the number of observation points for a single 6-hour period.

GEOS-5 SUPPORT OF NASA FIELD CAMPAIGNS: TC4 • ARCTAS • TIGERZ



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◀ Detail of Figure 2.

Project Description: Weather forecasts are an important part of planning aircraft flights for NASA's field campaigns, as is ancillary information such as aerosol distributions. A team at NASA Goddard Space Flight Center supports NASA field campaigns with real-time products and forecasts from the Goddard Earth Observing System Model, Version 5 (GEOS-5) to aid in flight planning and post-mission analysis. The objective is to provide a wide variety of mission-specific information on weather and atmospheric composition, summarized for ease of access through the Data Portal hosted by the NASA Center for Computational Sciences (NCCS). This support requires the close collaboration of mission planners and several organizations at NASA Goddard: the Global Modeling and Assimilation Office, the Atmospheric Chemistry and Dynamics Branch, the Software Integration and Visualization Office, and NCCS.

Three recent examples of GEOS-5 support for field campaigns were the TC4 (Tropical Composition, Cloud and Climate Coupling), ARCTAS (Arctic Research of the Composition of the Troposphere from Aircraft and Satellites), and TIGERZ missions. The TC4 mission, from July 12 to August 12, 2007, investigated atmospheric structure, properties, and processes in the tropical Eastern Pacific. The ARCTAS field campaign was undertaken during Spring and Summer 2008 to investigate the atmospheric transport pathways from mid-latitudes to the Arctic, and the relative contributions of different source regions to Arctic air pollution. Thus, for ARCTAS, the GEOS-5 system was instrumented with a set of tagged tracers to track transport: hydrophobic/hydrophilic organic carbon tag tracers driven by boreal and non-boreal biomass burning; carbon monoxide (CO) tag tracers driven by boreal and non-boreal biomass burning and by non-biomass emissions over Northern and Southern Asia, Europe, and North America; and chlorofluorocarbon (CFC) tag tracers with tropospheric and stratospheric origins. We determined biomass-burning sources of carbonaceous aerosols, CO, and sulfur dioxide (SO_2) in near real-time from MODIS imagery and land mapping. These were persisted forward in time for forecasts. We identified dust and sea-salt aerosol sources from the local meteorology, and specified other emissions from climatological databases. The ARCTAS system was continued during May and June 2008 to support the TIGERZ campaign, for which the AERONET (Aerosol Robotic Network) project deployed ground-based instruments to look at clouds and aerosols in the Indo-Gangetic basin.

Products for the field campaigns were based on meteorological analyses from the GEOS-5 data assimilation and forecast system. This system was complemented by the GEOS-5 Aerosol/Chemistry (AeroChem) components, including global CO and carbon dioxide (CO_2) tracers and aerosols (dust, sea-salt, organic carbon, black carbon, and sulfates) from the Goddard Chemistry Aerosol Radiation and Transport (GOCART) model. We provided the analyses and 5-day forecasts to the flight-planning teams in near real-time. Examples of meteorological and aerosol/chemical products available through a multi-faceted data delivery system can be found at http://gmao.gsfc.nasa.gov/projects/arctas/.

Relevance of Work to NASA: NASA undertakes aircraft field campaigns as part of its science mission strategy. These campaigns integrate satellite and aircraft observations for scientific analysis and satellite algorithm validation. GEOS-5 analyses and forecasts are one of the information sources used by satellite and model science teams in pre-mission flight planning and post-mission data interpretation. This work is funded by NASA's Modeling, Analysis, and Prediction (MAP) Program.

Computational Approach: GEOS-5 uses finite-volume dynamics on a spherical grid. The configuration used for these field campaigns has a 2/3-degree longitude by 1/2-degree latitude grid with 72 vertical levels to 0.01 hectopascals (hPa), with assimilation analyses conducted every 6 hours. The analysis uses a three-dimensional variational approach to solve the least-squares fit of GEOS-5 analysis states to the model (background) states and to the available satellite and *in situ* data. Advection, diffusion, and convective transport of the CO, CO_2, and GOCART tracers are performed on-line within GEOS-5. For TC4, we conducted an additional ¼-degree 2-day meteorological forecast to aid flight planning.

Results: Figures 1 and 2 show examples of GEOS-5 products for ARCTAS. The mission support was successful, with GEOS-5 products delivered on time for most of the mission duration thanks to the NCCS ensuring timely execution of job streams and supporting the data portal. For example, a DC-8 flight on June 29, 2008 sampled the Siberian fire plume transported to the region in the mid-troposphere as predicted by GEOS-5.

Role of High-End Computing: The GEOS-5 systems were run on 128 processors of the NCCS Explore supercomputer, with a continuous job stream allowing timely delivery of products to inform flight planning.

Future: GEOS-5 products with improved systems (e.g., the ARCTAS system was updated from the TC4 system) will be used for post-mission analysis. The system will also be used to support HIPPO (High-performance Instrumented Airborne Platform for Environmental Research [HIAPER] Pole-to-Pole Observations), a mission that will measure cross-sections of atmospheric concentrations approximately pole-to-pole from the surface to the tropopause. The program will provide the first comprehensive, global survey of atmospheric trace gases, covering the full troposphere in all seasons and multiple years. We will also support other field campaigns as they arise.

Co-Investigators

- Peter Colarco, Arlindo da Silva, Max Suarez, Ricardo Todling, Larry Takacs, Gi-Kong Kim, Eric Nielsen, all of NASA Goddard Space Flight Center

Publications

[1] Rienecker, M.M., et al., "The GEOS-5 Data Assimilation System – Documentation of Versions 5.0.1, 5.1.0 and 5.2.0," *NASA GSFC Technical Report Series on Global Modeling and Data Assimilation*, NASA/TM-2008-104606, Vol. 27, 101 pp, 2008.

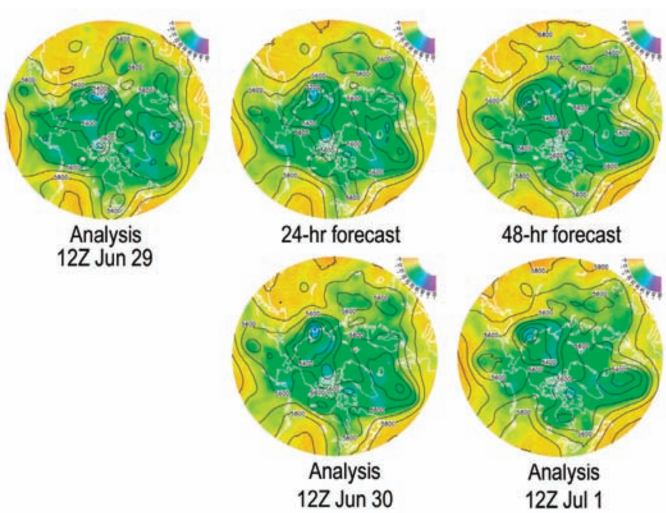

Figure 1: This image shows 500-hectopascal (hPa) temperatures (shading) and heights (contours) during NASA's ARCTAS (Arctic Research of the Composition of the Troposphere from Aircraft and Satellites) mission. An analysis from the Goddard Earth Observing System Model, Version 5 (GEOS-5) is shown with 24- and 48-hour forecasts and validating analyses. These fields, with the accompanying atmospheric chemistry fields, were used to help plan a DC-8 flight on June 29, 2008.

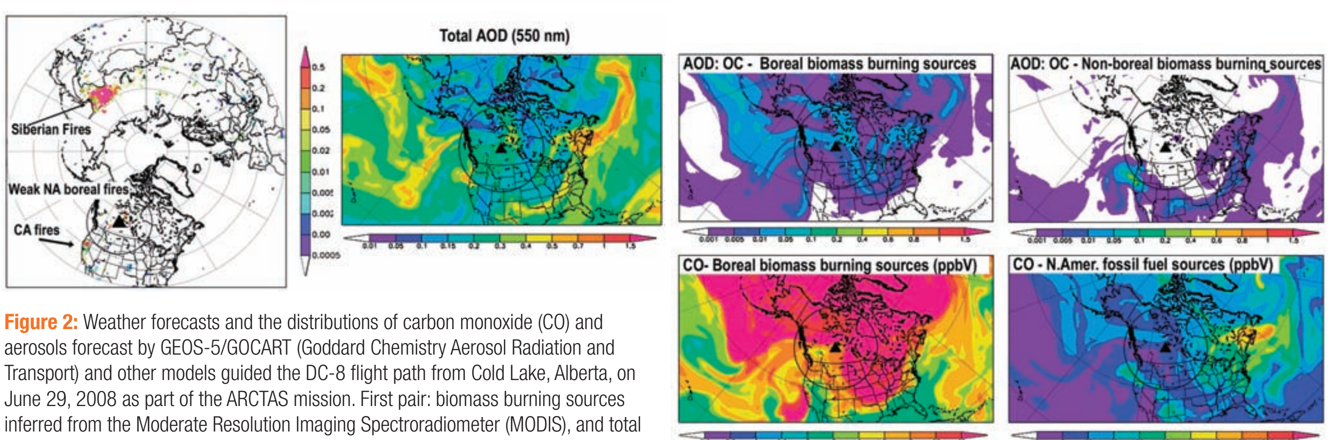

Figure 2: Weather forecasts and the distributions of carbon monoxide (CO) and aerosols forecast by GEOS-5/GOCART (Goddard Chemistry Aerosol Radiation and Transport) and other models guided the DC-8 flight path from Cold Lake, Alberta, on June 29, 2008 as part of the ARCTAS mission. First pair: biomass burning sources inferred from the Moderate Resolution Imaging Spectroradiometer (MODIS), and total column aerosol optical depth (AOD) at 550 nanometer (nm) wavelength. Second pair: AOD contributions from boreal and non-boreal biomass emissions. Third pair: CO distributions (parts per billion by volume, ppbV) at 550 hPa from boreal biomass burning and North American fossil fuel emissions.

GLOBAL MODELING OF AEROSOLS AND THEIR IMPACTS ON CLIMATE AND AIR QUALITY

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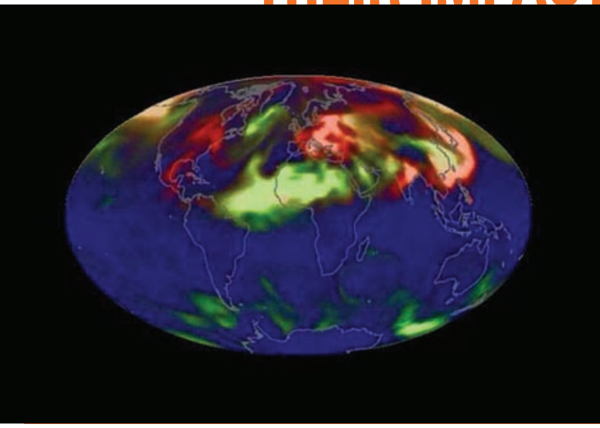

◄ Snapshot from Figure 1.

Project Description: We have several projects supported by NASA's Science Mission Directorate, with an overall goal to develop a global aerosol/chemistry/transport model to study aerosols and their impacts on climate and air quality, through the use and analysis of satellite and other observational data. We seek to understand the role of aerosols in radiative forcing and climate change from pre-industrial time to the present, and to investigate regional and global change of aerosols and related gases over multi-decadal time-scales. We are also assessing the effect of long-range aerosol transport and anthropogenic emissions on surface air quality, as well as supporting NASA field experiments and satellite retrievals.

Collectively, our research projects focus on interactive use of the Goddard Chemistry Aerosol Radiation and Transport (GOCART) model alongside satellite and *in situ* observations. We use satellite-based fire data to improve simulations of biomass burning emissions and land-cover/vegetation data to account for dust source variations. We use the model to conduct multi-year simulations of aerosols and trace gases, which we compare with data from NASA's satellites and sensors, including the Moderate Resolution Imaging Spectroradiometer (MODIS), Multiangle Imaging SpectroRadiometer (MISR), Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observation (CALIPSO), Ozone Monitoring Instrument (OMI), Measurements of Pollution in the Troposphere (MOPITT), and Atmospheric Infrared Sounder (AIRS).

We investigate the relationships between aerosols and carbon monoxide (CO) in terms of sources, chemistry, and long-range transport. We calculate the aerosol radiative forcing and estimate its climate effects in different regions.

In addition, we evaluate the application of satellite data to air quality studies by examining the quantitative link between the remotely sensed data and surface pollutant concentrations and testing the applicability of combining aerosols with CO. We also provide model information on aerosol composition and vertical distributions to satellite retrieval teams.

Relevance of Work to NASA: Our projects are supported by several NASA programs, including the Modeling, Analysis, and Prediction (MAP) Program; the Atmospheric Composition Modeling and Analysis Program (ACMAP); the Earth Observing System (EOS); CALIPSO; and the Tropospheric Chemistry Program (TCP). Our activities are highly relevant to NASA's science objectives, particularly to understanding the mechanisms that drive Earth system changes and the Earth system's response to natural and human-induced changes.

Computational Approach: GOCART is a global model of atmospheric processes, including emission, chemistry, dry deposition, wet removal, advection, convection, and radiative forcing. Our projects use supercomputing for many model runs of different scenarios.

Results:

- *Intercontinental transport of aerosols and implications for regional air quality:* This study assesses the impact of long-range transport of aerosols (Figure 1).
- *Possibilities and challenges in using satellite aerosol optical depth (AOD) data for air quality studies:* This study investigates the relationship of column AOD to surface concentrations of fine-grained ($PM_{2.5}$) airborne particulate matter.
- *Aerosol absorption:* Aerosol absorption is a key parameter for estimating the climate forcing of aerosols. This project examines the global distribution of absorbing aerosols and compares the quantities from NASA's ground-based Aerosol Robotic Network (AERONET) (Figure 2).
- *Long-term trend of atmospheric aerosols:* This project simulates global aerosol changes from 1980 to the present and examines the relationship between emission, atmospheric loading, and AOD.

Role of High-End Computing: Our research critically depends on the NASA Center for Computational Sciences (NCCS), whose supercomputers have performed all the simulations, and whose personnel have helped our group to optimize model executions and to transition from one platform to another.

Future: We aim to conduct global model simulations at much higher spatial and temporal resolutions and spanning multiple decades; our computing needs will grow significantly.

Co-Investigators

- Thomas Diehl, Huisheng Bian, Hongbin Yu, Qian Tan, Tom Kucsera, all of NASA Goddard Space Flight Center/University of Maryland, Baltimore County

Publications

[1] Chin, M., Diehl, T., Ginoux, P., and Malm, W., "Intercontinental Transport of Pollution and Dust Aerosols: Implications for Regional Air Quality," *Atmospheric Chemistry and Physics*, Vol. 7, pp. 5501–5517, 2007.

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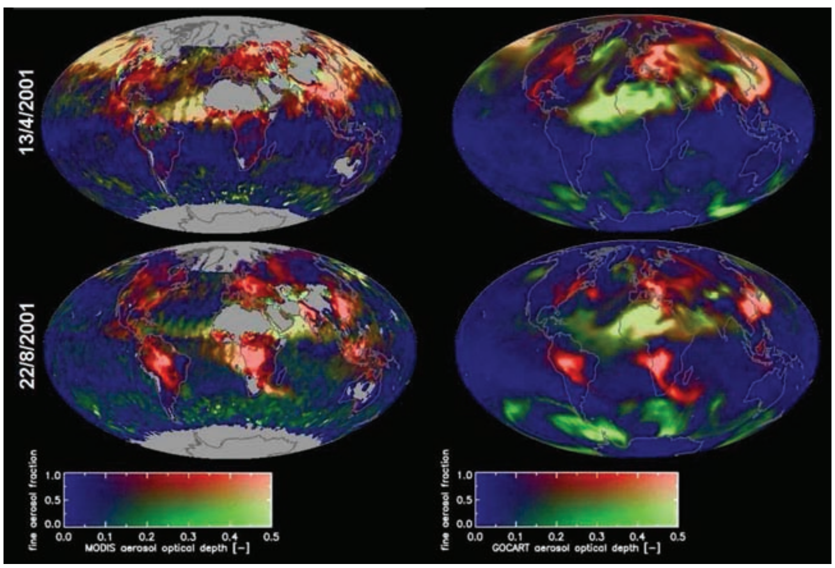


Figure 1: Aerosol optical depth observed by the Moderate Resolution Imaging Spectroradiometer (MODIS) (left) and simulated by the Goddard Chemistry Aerosol Radiation and Transport (GOCART) model (right) for 13 April 2001 (top) and 22 August 2001 (bottom). Red indicates fine mode aerosols (e.g., pollution and smoke); green indicates coarse mode aerosols (e.g., dust and sea-salt); color brightness is proportional to the aerosol optical depth. 13 April sees transport of heavy dust and pollution from Asia to the Pacific, and dust transport from Africa to the Atlantic. 22 August sees large smoke plumes over South America and Southern Africa.

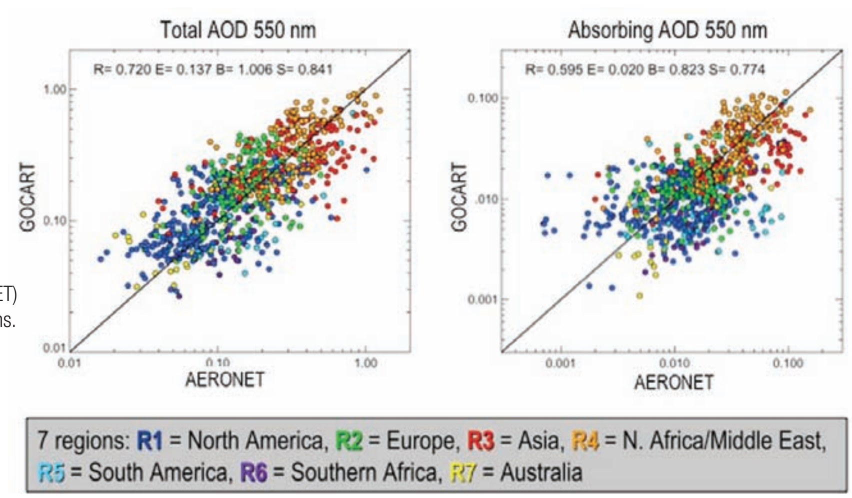
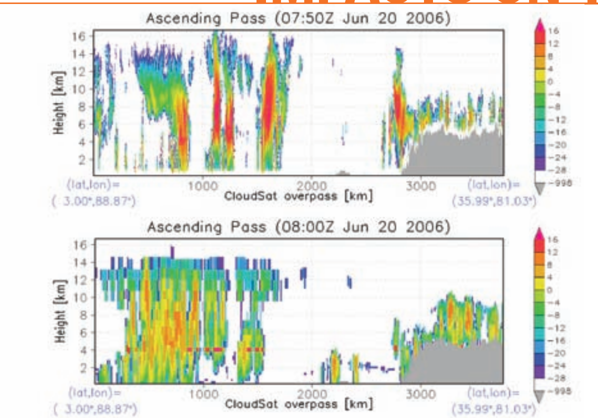


Figure 2: Comparisons of total (left) and absorbing (right) aerosol optical depth from Aerosol Robotic Network (AERONET) observations and GOCART simulations in seven global regions. Data are monthly averaged values in 2004.

HIGH-RESOLUTION MODELING OF AEROSOL IMPACTS ON THE ASIAN MONSOON WATER CYCLE



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◀ **Figure 1:** Cross-sections of radar echo observed by the CloudSat Cloud Profiling Radar (top) and simulated by the Weather Research and Forecasting (WRF) Model (bottom) for June 20, 2006. The model echoes are based on the Satellite Data Simulation Unit (SDSU) radar simulator. Units are in dBZ, a measure of reflectivity.

Project Description: Severe floods and droughts caused by monsoon fluctuations have always impacted Asian societies. As monsoons now interact with aerosols from industrial and urban pollution, they threaten the water supply, human health, and biodiversity of the Asian monsoon region. This interaction may also exacerbate the global effects of climate change, given the region's dense population and its role in the global water cycle.

This project aims to clarify the interactions between aerosols and the monsoon water cycle, and how they may modulate the regional climatic impacts of global warming. The project is testing various feedback hypotheses using high-resolution climate models and satellite and *in situ* observations.

We are using the regional-scale Weather Research and Forecasting (WRF) Model to simulate the impacts of absorbing aerosols (dust and black carbon) on the Indian monsoon water cycle and to test several hypotheses [5, 6]. Thanks to its flexible horizontal and vertical resolution, WRF can realistically represent a wide range of physical processes, topography, radiative transfer, precipitation and cloud processes, and land/atmosphere hydrology and energy coupling. We have implemented a radiation module that computes short- and long-wave radiative flux and atmospheric heating. This scheme links to the Goddard Chemistry Aerosol Radiation and Transport (GOCART) aerosol module to estimate aerosol concentrations, optical depth, optical properties, and effects on cloud-precipitation microphysics, structure, and dynamics.

Relevance of Work to NASA: With funding from the Earth Science Division's Interdisciplinary Investigation Program, this work serves NASA's goal to understand climate change impacts on the water cycle. It uses satellite products from NASA's Tropical Rainfall Measuring Mission (TRMM), Moderate Resolution Imaging Spectroradiometer (MODIS), CloudSat, and Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observation (CALIPSO) and outputs from a NASA chemistry transport model to construct aerosol-forcing functions and validate model results.

Computational Approach: In order to resolve the microphysics of cloud and rain formation, we run WRF at very high resolution—less than 10-kilometer (km) horizontal grid spacing with 31 vertical layers. To mitigate the large computational demand, we use a triple-nest grid with horizontal resolutions of 27, 9, and 3 km. Using the Discover supercomputer at the NASA Center for Computational Sciences, we conducted a model integration for the period May 1 to July 1 (covering the pre-monsoon and the monsoon onset) in both 2005 and 2006. This provides a good case study, as observations show heavier loading of absorbing aerosols (dust and black carbon) in 2006.

Results: We recently documented the "elevated-heat-pump" (EHP) hypothesis linking aerosols to the monsoon cycle; this highlights the role of the Himalayas and Tibetan Plateau in trapping aerosols over the Indo-Gangetic Plain. Studies using satellite and reanalysis data show preliminary evidence of aerosol impacts on the variability of the Indian monsoon. We have also implemented the radiative codes associated with different aerosol species, so that we can use the model to study the impacts of aerosol forcing. And through control and anomalies experiments, we have tested the model's sensitivity to the domain design and the cumulus parameterization, and ensured implementation of the proper aerosol radiation codes.

In the 2005/6 model integration, simulated cloud vertical profiles compare fairly well with CloudSat observations (Figure 1), and simulated rainfall agrees reasonably well with daily rainfall distribution (Figure 2), producing heavy rain (red) over the Bay of Bengal and the western coast. Preliminary results show significant promise for the WRF-GOCART module in studying aerosol effects on the monsoon cycle.

Role of High-End Computing: A cloud-resolving mesoscale model is computationally demanding; our model domain contains over 200,000 grid cells. By using 256 Intel Xeon processors on Discover, we can finish a 1-day integration in less than 3 hours. The challenge now becomes data migration or transfer, as network bandwidths have not kept pace with computing speeds.

Future: We expect to complete the first integration for the two simulated months over WRF simulation Domains 1 (27-km grid) and 2 (9-km grid), using several schemes for aerosol forcing and cumulus parameterization. We will then carry out a 2-week model integration using Domain 3 (3-km grid) to examine diurnal variability, orographic effects, and possible microphysics effects on land convection immediately before and after the monsoon onset. We expect model outputs on the order of 50 terabytes.

Co-Investigators

- Wei-Kuo Tao, Mian Chin, NASA Goddard Space Flight Center
- Kyu-Myong Kim, Jainn J. (Roger) Shi, Toshihisa Matsui, all of University of Maryland, Baltimore County

Publications

[1] Gautam, R., Hsu, N.C., Kafatos, M., Tsay, S.-C., "Influences of Winter Haze on Fog/Low Cloud over the Indo-Gangetic Plains," *Journal of Geophysical Research*, Vol. 112, D05207, doi:10.1029/2005JD00703, 2007.

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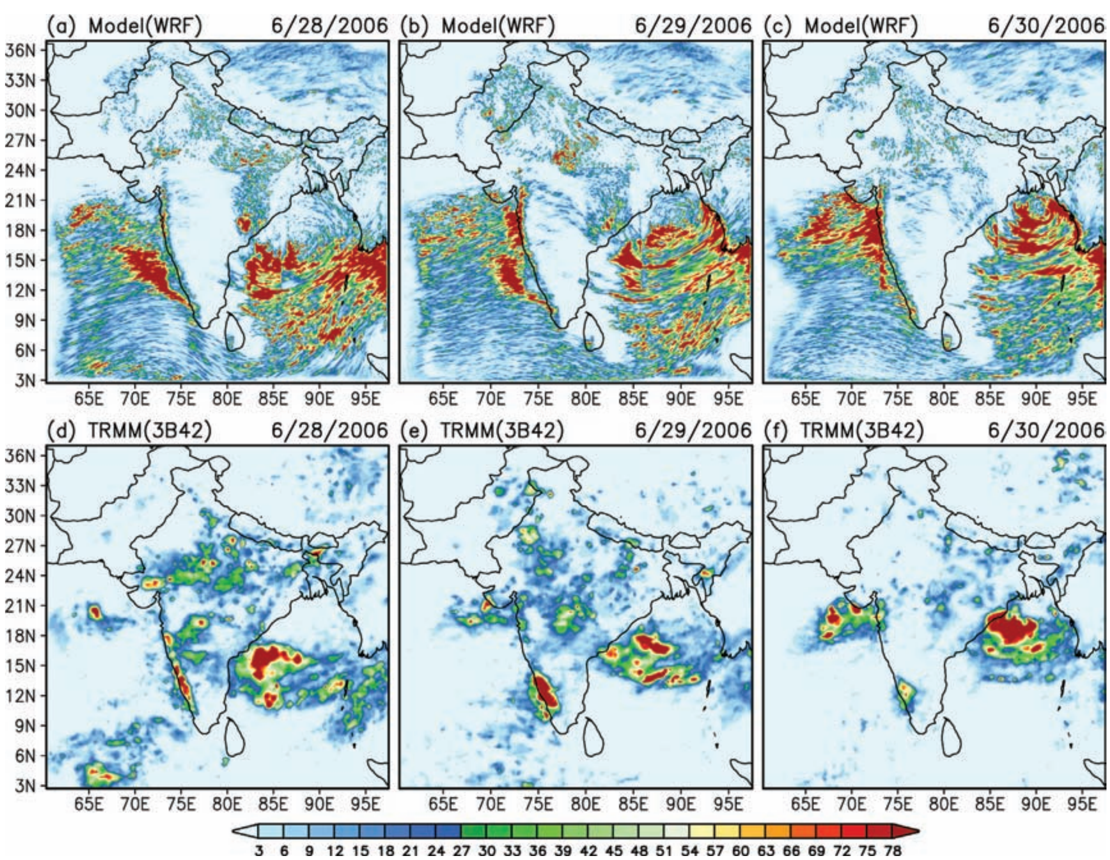
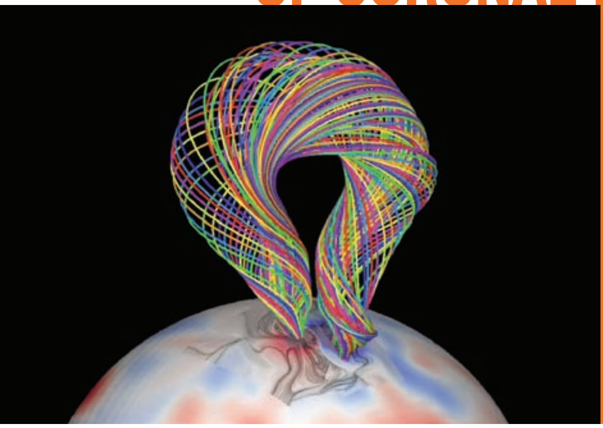


Figure 2: Rainfall distributions from Weather Research and Forecasting (WRF) Model simulations at 9-kilometer resolution (top row) and from Tropical Rainfall Measurement Mission (TRMM) satellite estimates (bottom row). Units are in millimeters per day.

HIGH-RESOLUTION SIMULATIONS OF CORONAL MASS EJECTIONS



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◀ Detail from Figure 1.

Project Description: Coronal mass ejections (CMEs) are violent eruptions that send giant clouds of solar plasma into space. The radiation and energetic particles from the solar flares that frequently accompany CMEs can cripple satellites, disrupt communications and power systems, and endanger humans in space. We believe that we can best understand the mysterious properties of CMEs using numerical simulations of solar magnetic fields. Models have matured enough that we can use them to interpret CME observations; understand the complex behavior of the Sun, especially the structure of the high-temperature corona and the dynamic events that occur within it; and determine how that structure and those events flow outward and manifest themselves in the surrounding heliosphere.

We are using numerical simulations of the solar corona to investigate what powers CMEs, how they are initiated, and how they propagate in the inner heliosphere. This task requires the development of detailed models of the corona and solar wind. We use "event studies" of CMEs in which we apply models that are as realistic as possible to make direct comparisons between models and observations. A long-term goal is to improve our ability to predict when flares and CMEs will occur. Such predictions are necessary for undertaking NASA's Vision for Space Exploration.

Relevance of Work to NASA: A central goal of NASA's Heliophysics program is to understand the influence of the Sun and its activity on the inner heliosphere. Present and upcoming NASA missions—including the Solar and Heliospheric Observatory (SOHO), Hinode, the Solar Terrestrial Relations Observatory (STEREO), and the Solar Dynamics Observatory (SDO)—produce massive quantities of high-resolution observations of the Sun. We need sophisticated 3D numerical models to interpret these data and, in turn, understand solar physics. Understanding CMEs, including their initiation, propagation, and interaction with the Earth's magnetosphere, is a central goal of the National Space Weather Program, which aims to protect the nation's space assets. Funding for this research comes from NASA's Heliophysics Theory and Living With a Star (LWS) Programs.

Computational Approach: We use 3D magnetohydrodynamic (MHD) numerical models to simulate in detail how the magnetic field of the Sun behaves. Our simulations use tens of millions of mesh points and tens of thousands of time-steps to evolve the solar magnetic field. Our 3D code uses implicit time-differencing, requiring iterative solvers to invert the resulting very large sparse matrices.

Results: We have been able to simulate the initiation and propagation of a CME from an active region observed on May 12, 1997, including its signature in extreme ultraviolet (EUV) and X-ray emissions (Figure 1). The simulated and observed CMEs have strikingly similar characteristics. We studied the topology of the magnetic field in detail to understand the role of magnetic reconnection in the eruption process. We have embarked on a new event study of the May 13, 2005 CME as part of a Focused Science Team for NASA's LWS Program. We have also predicted the structure of the solar corona for the August 1, 2008 total solar eclipse (Figure 2). These studies are crucial tests of the model's predictive capability and give us important clues on how to improve the model. A version of our 3D code, Magnetohydrodynamics outside A Sphere (MAS), is available to the heliophysics community through NASA's Community Coordinated Modeling Center (CCMC).

Role of High-End Computing: We need massively parallel supercomputers such as Columbia at the NASA Advanced Supercomputing (NAS) facility to solve the stiff equations that describe the evolution of magnetic fields on the Sun. Our code uses domain decomposition and runs particularly well on the fast-communication interconnect on Columbia using the standard Message Passing Interface (MPI). The code works on a wide variety of architectures and scales well on thousands of processors. It is suitable for transition to the next generation of massively parallel petascale machines.

Future: The high-resolution images that will come from NASA's SDO mission will require simulations with even more mesh points. In addition, SDO's multi-spectral observations will provide opportunities to improve our understanding of coronal heating mechanisms by comparing models with EUV and X-ray emission observations. We plan to continue to improve our model to meet these challenges.

Co-Investigators

- Jon A. Linker, Pete Riley, Roberto Lionello, Viacheslav Titov, all of Predictive Science, Inc.
- Yung Mok, University of California, Irvine

Publications

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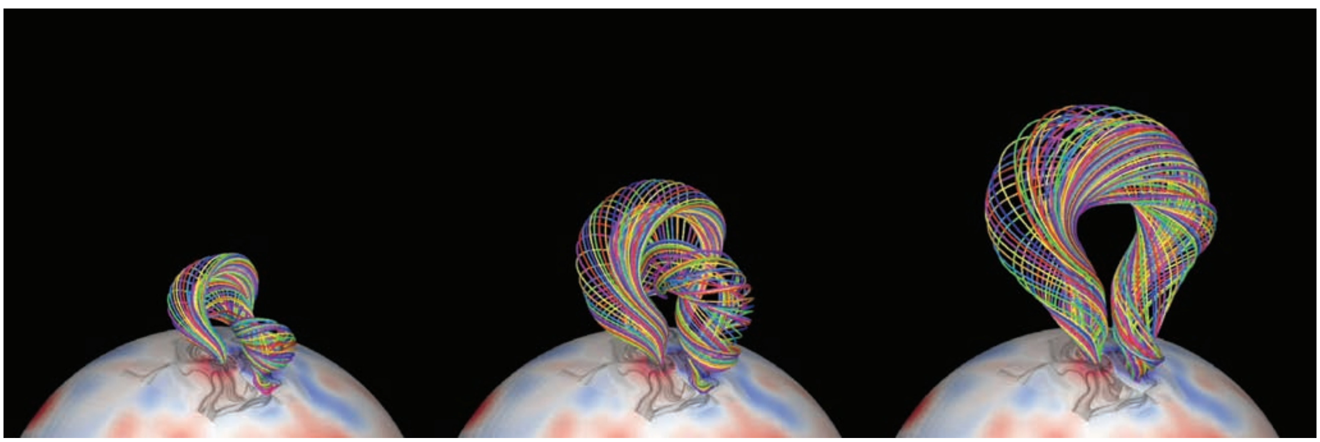


Figure 1: A numerical simulation of the eruption of a coronal mass ejection from the Sun on May 12, 1997. The magnetic field lines show a flux rope that eventually becomes an interplanetary magnetic cloud, which was observed at Earth.

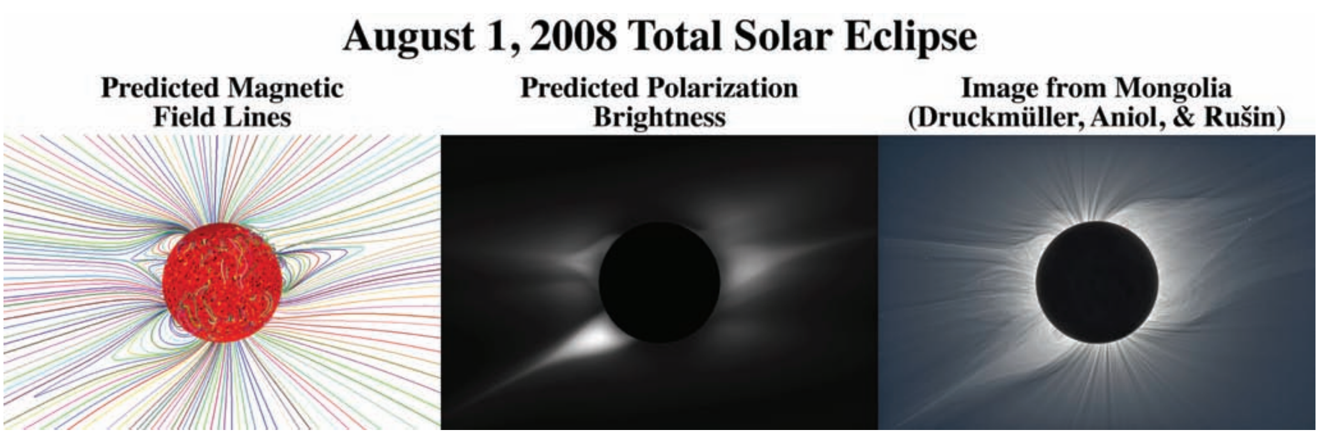
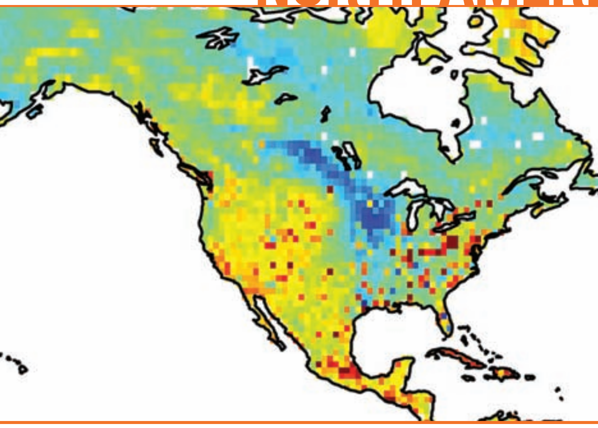


Figure 2: The August 1, 2008 total solar eclipse corona as predicted by a magnetohydrodynamic (MHD) model and as observed from Bor Udzuur, Mongolia.

HIGH-RESOLUTION WIND FIELDS FOR CONSTRAINING NORTH AMERICAN FLUXES OF CARBON DIOXIDE



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◀ Close-up of Figure 2.

Project Description: Our work is part of an ongoing project entitled *Constraining North American Fluxes of Carbon Dioxide and Inferring Their Spatiotemporal Covariances through Assimilation of Remote Sensing and Atmospheric Data in a Geostatistical Framework*, funded through NASA's North American Carbon Program (NACP). The overall goal is to use remotely sensed and atmospheric data in a geostatistical inverse modeling framework to quantify North American sources and sinks of carbon dioxide (CO_2) with unprecedented spatial and temporal resolution. Using the Columbia supercomputer at the NASA Advanced Supercomputing (NAS) facility, we are producing high-resolution meteorological fields with the Weather Research and Forecasting (WRF) atmospheric model, and using these to drive the Stochastic Time-Inverted Lagrangian Transport (STILT) atmospheric transport model and calculate the sensitivity of atmospheric CO_2 measurements to surface fluxes.

This project will address the NACP's stated goals of (i) developing quantitative scientific knowledge, robust observations, and models to determine emissions and uptake of CO_2 and the factors regulating these processes, and (ii) developing the scientific basis to implement full carbon accounting, including natural and anthropogenic fluxes of CO_2 on regional and continental scales. We will achieve our goal of quantifying CO_2 surface fluxes without relying on *a priori* flux estimates, while rigorously quantifying the magnitude and spatiotemporal covariance of the various components of model, measurement, and flux errors. In addition, we will evaluate the sensitivity of the inferred fluxes to available remotely sensed environmental datasets, providing the process-based understanding needed to improve bottom-up inventories and biospheric models, thereby enabling more accurate flux accounting.

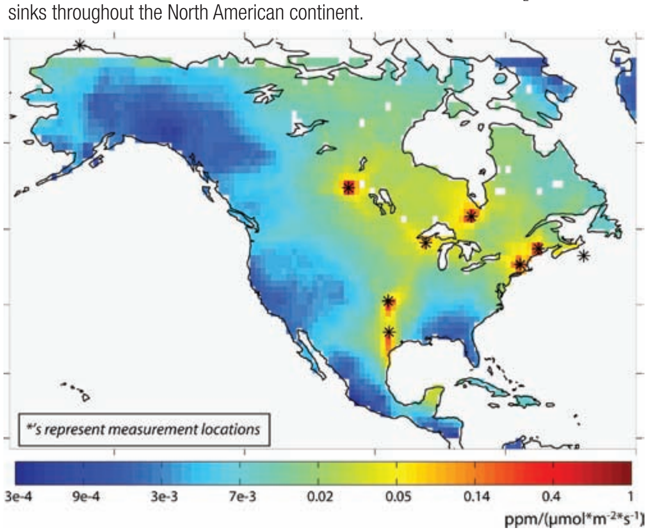
Relevance of Work to NASA: The NACP implementation plan calls for the development, demonstration, and evaluation of inverse techniques for estimating monthly CO_2 exchange on a 100-km grid from atmospheric observations. We address this need by merging available atmospheric measurements of CO_2 with NASA remote-sensing data to estimate fluxes of CO_2 directly at high spatiotemporal resolutions, without relying on prior estimates of flux distributions. The project also presents a significant opportunity to use NASA's spatially distributed satellite observations of the Earth to improve our understanding of the North American carbon budget.

Computational Approach: In order to resolve mesoscale circulation, cloud venting, and other detailed atmospheric phenomena that affect CO_2 transport, the WRF model is nested down to high resolution (2 km) over target regions surrounding tall towers with continuous, long-term, hourly monitoring of CO_2 concentrations in Wisconsin, Maine, and Texas. The 2-km domain is the innermost grid; it is embedded within a 10-km grid domain over the Eastern United States, and an outermost 40-km grid domain covering Mexico, the U.S., and Canada. Two-way nesting allows the dynamics simulated within the innermost nest to propagate outward into coarser nests. The WRF model is forced at the lateral boundaries by meteorological fields from the National Centers for Environmental Prediction (NCEP) North American Regional Reanalysis, which has already assimilated an extensive array of atmospheric observations from radiosondes, satellites, and ground stations. These fields are also used for analysis nudging of the outermost domain. The nested WRF windfields contain much more fine-scale information than the 2-degree (or coarser) products used by typical inverse modeling studies, or readily available regional analysis fields typically at 40-km resolution. The WRF fields produced from this study will be freely available to the carbon community.

Results: We began using the NAS Columbia system actively in spring 2007. Since that time, we have generated nested meteorological fields for 2004, 2005, 2006, and 2007. In spring 2008, we began experimenting with the STILT model on Columbia to quantify the sensitivity of available measurements of atmospheric CO_2 to terrestrial fluxes at a 1-degree resolution for the North American continent (Figures 1 and 2). We are now using the system to run STILT for all years for which meteorological fields have been generated.

Role of High-End Computing: Columbia has enabled us to create an unprecedented dataset of meteorological fields for 2004 to 2007 using the WRF model, a well-established community mesoscale modeling framework that supports multiple dynamical cores, numerical schemes, and physical parameterization packages. The software framework has built-in support for parallel architectures. Specifically, we use the Advanced Research WRF (ARW) supported by the National Center for Atmospheric Research. The ARW is a finite-difference code using 3rd-order Runge-Kutta time-stepping. Physics packages are available for the treatment of soil, surface, boundary layer, moist physics, and radiative processes.

Figure 1: Sensitivity of measurements available in June 2004 to CO_2 sources and sinks throughout the North American continent.



Future: Our work focuses on quantifying the sensitivity of available continuous measurements of atmospheric CO_2 to North American CO_2 fluxes at fine spatiotemporal resolutions. We expect this work to continue for the upcoming year. Through ongoing collaborations, we plan ultimately to create a 5-year record of meteorology, atmospheric transport, and estimated fluxes.

Co-Investigators

- Adam I. Hirsch, University of Colorado and NOAA Earth System Research Laboratory
- Thomas Nehrkorn, Atmospheric and Environmental Research, Inc.
- John C. Lin, University of Waterloo

Publications

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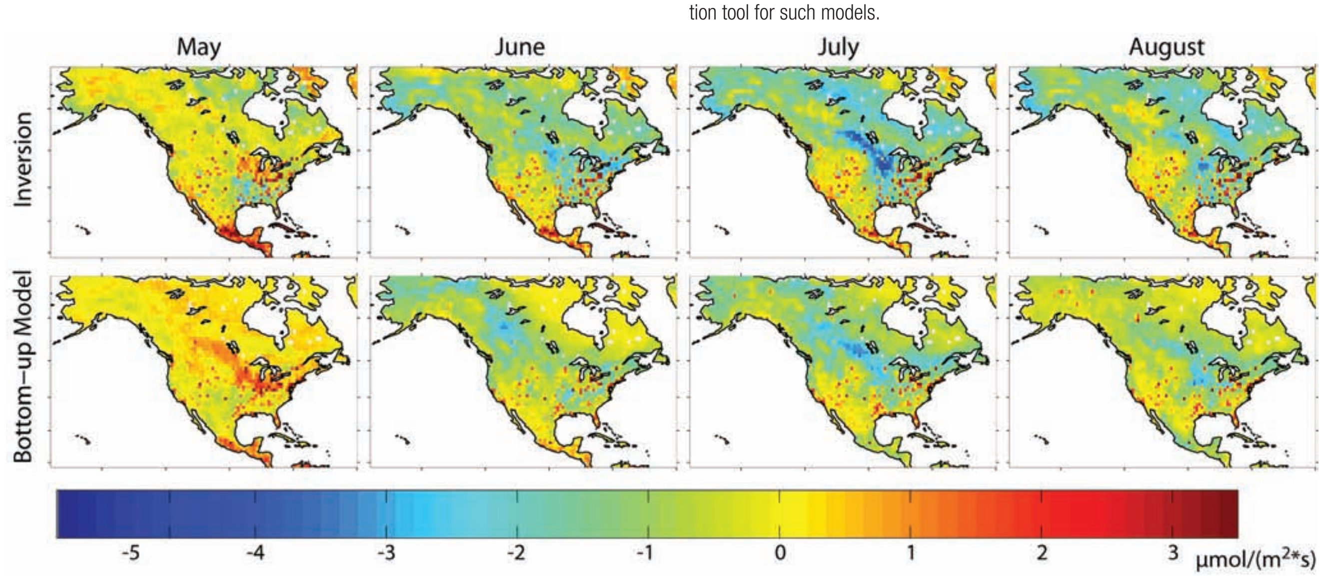
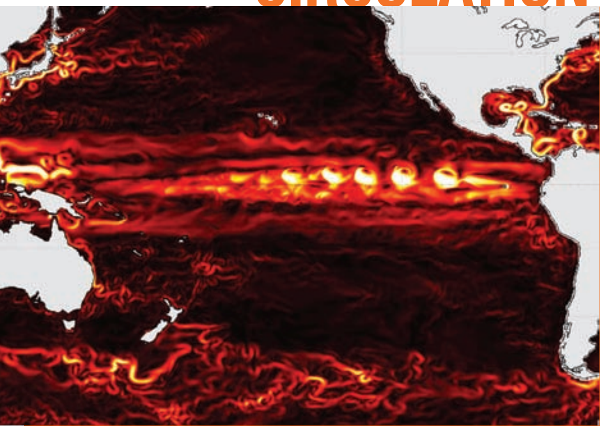
Figure 2: Top row: monthly grid-scale CO_2 flux estimates for 2004 resulting from the North American geostatistical inversion. In addition to atmospheric measurements and transport information, investigators incorporated several Moderate Resolution Imaging Spectroradiometer (MODIS)-derived data products, climate parameters, and fossil fuel inventories into the inversion. Bottom row: for comparison, grid-scale flux estimates derived from bottom-up or mechanistic models (the Carnegie-Ames-Stanford Approach [CASA] biospheric model, fire emissions, and fossil fuel inventories) are also presented. Because the geostatistical inversion does not make use of bottom-up models, inversion results can also serve as an evaluation tool for such models.



NON-BOUSSINESQ OCEAN GENERAL-CIRCULATION MODEL AND GRACE APPLICATIONS



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◀ Close-up of Figure 1.

Project Description: With funding from NASA's Modeling, Analysis, and Prediction (MAP) Program, we are modeling global ocean-ice circulation and validating the results with data from the Gravity Recovery and Climate Experiment (GRACE) satellites. Our goal is to develop an advanced mass-conserving (Non-Boussinesq) ocean general-circulation model (OGCM), allowing use of satellite data for a better understanding of the ocean's climate. The scientific objectives are threefold:

- Compare GRACE, Earth rotation, and other geodetic observations with mass-conserving models from the NASA Jet Propulsion Laboratory (JPL) to improve NASA's next-generation assimilation system.
- Quantify the dynamic balance of wind-stress curl and bottom-pressure torque by using wind data from NASA's Quick Scatterometer (QuikSCAT), bottom-pressure data from GRACE, and simulation products from NASA's Global Modeling and Assimilation Office.
- Study ocean-solid-Earth interactions and global sea-level changes by applying geodetic observations to the climate model system.

The global ocean-ice model is designed to better represent ocean mass variation and the effect of topography on ice-shelf flows. Our coupled ocean-ice system includes a dynamic-thermodynamic sea-ice component based on an elastic-viscous-plastic rheology. The ocean and ice models communicate by the exchange of heat, fresh water, and momentum at the ocean-ice interaction layer. The water depth of the model is divided into 30 terrain-following, stretched-pressure levels from shallow coast to the deep ocean [1]. Topography data is from ETOPO2 with modification from the Navy's DBDB2 bathymetry to give special care to strait geometry when generating the model grid. The model is spun up for 30 years with an annual mean forcing to reach an approximate steady state, and then driven by daily National Centers for Environmental Prediction (NCEP)/National Center for Atmospheric Research (NCAR) reanalysis forcing from 1970 to the present. With the northern pole displaced towards Russia, the mass-conserving ocean and ice model has included both polar regions. A snapshot of the model ice concentration and ocean circulation is shown in Figure 1.

Relevance of Work to NASA: This project will provide an improved picture of ocean bottom pressure and its dynamic link to sea-surface height and geodetic observations. This will provide a direct comparison with GRACE and Earth rotation observations as well as insights into the determination and interpretation of global sea-level change. The derived ocean and ice data will be made available on-line (http://earthquake-tsunami.jpl.nasa.gov). The synergistic applications of the satellite data should provide insights to addressing NASA's research strategy questions: "How is the global ocean circulation varying on interannual, decadal, and longer time scales?," "How can climate variations induce changes in global ocean circulation?," and "How is global sea-level affected by climate change?"

Computational Approach: The global ocean and ice model is modular Fortran 90 and Fortran 95 code. It uses C preprocessing to activate the physical and numerical options. We have established several coding standards to facilitate model readability, maintenance, and portability. All the state model variables are dynamically allocated and passed as arguments to the computational routines via de-referenced pointer structures. All private or scratch arrays are automatic; their size is determined when the procedure is entered. This code structure facilitates computations over nested and composed grids.

Results: We have completed three tasks: (i) compared model ocean-bottom-pressure results with GRACE observations (Figure 2); (ii) carried out coupled earthquake-OGCM simulations for the 2004 Indian Ocean tsunami [2, 3]; and (iii) coupled a sea-ice model into the OGCM [4–7].

Role of High-End Computing: The parallel framework is coarse-grained, with both shared- and distributed-memory paradigms coexisting in the same code. The code has extensive pre- and post-processing software for data preparation, analysis, plotting, and visualization. All model input and output is via NetCDF, which facilitates the interchange of data between computers, user communities, and other independent analysis software. The speed and parallel capabilities of NASA's High-End Computing facilities are crucial to the project.

Future: We plan to couple and develop an ice-sheet model with JPL's OGCM for a better understanding of ocean-ice interactions, ice-shelf/ice-sheet/glacier melting, and their impact on oceanic climate and sea-level rise. We also plan to consider both polar regions in assessing mass exchanges between the cryosphere and oceans with data from GRACE and ICESat (Ice, Cloud, and land Elevation Satellite)—which measure ice-sheet and glacier mass balance and sea-ice thickness change.

Co-Investigators

- Richard Gross, Victor Zlotnicki, NASA Jet Propulsion Laboratory
- C.K. Shum, Ohio State University
- Dale Haidvogel, Rutgers University

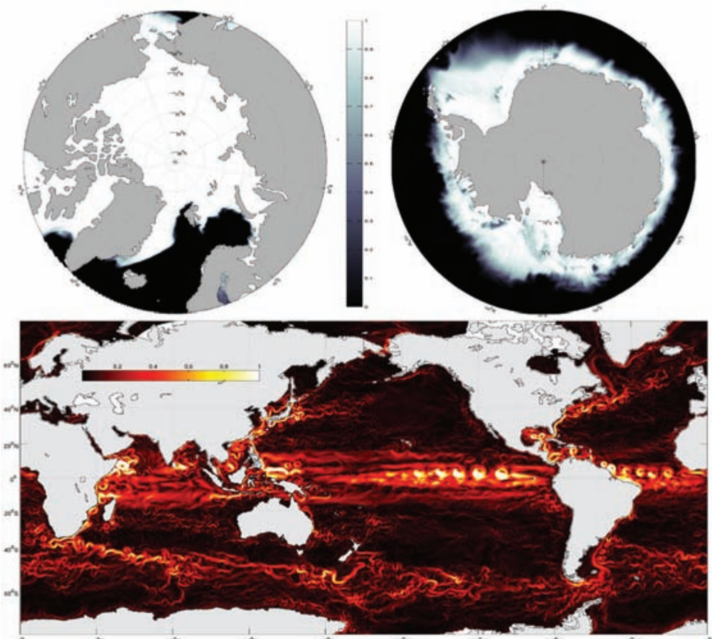

Figure 1: Coupled ocean-ice model for the global ocean. The top panels show simulated ice concentration in the Arctic and Antarctic regions. The bottom panel shows speeds of simulated ocean currents. In this projection, the model's north pole is shifted towards Russia to avoid the computational singularity.

Publications

[1] Song, Y.T., and Hou, T.Y., "Parametric Vertical Coordinate Formulation for Multiscale, Boussinesq, and Non-Boussinesq Ocean Modeling," *Ocean Modelling*, Vol. 11, Nos. 3–4, pp. 298–332, Doi:10.1016/j.ocemod.2005.01.001, 2006.

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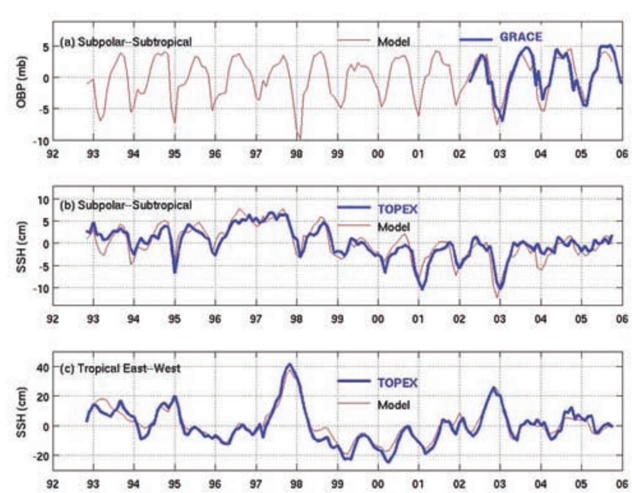
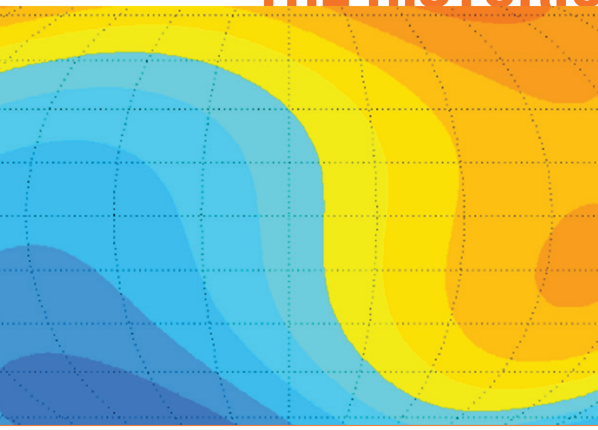


Figure 2: Comparison of the ocean model with observed data from 1993 to 2006. The top panel shows simulated ocean-bottom-pressure variability compared with Gravity Recovery and Climate Experiment (GRACE) observations of the ocean in the subpolar-subtropical regions. The middle and bottom panels show simulated sea-surface heights compared with TOPEX/Poseidon observations of the Pacific Ocean in the subpolar-subtropical and tropical east-west regions.

NUMERICAL SIMULATION OF THE HISTORICAL MARTIAN DYNAMO



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◀ Detail of Figure 1.

Project Description: The Mars Global Surveyor's detection of a Martian magnetic anomaly suggests that Mars once possessed an active, global, internal magnetic field that was generated and maintained by convective flow in an electrically conducting fluid core (dynamo). It also appears that the dynamo action lasted for only several hundred million years after the accretion of the planet.

We aim to understand the Martian dynamo and its termination by means of large-scale numerical simulations with the *m*MoSST (Message Passing Interface (MPI)-based, Modular, Scalable, Self-consistent and Three-dimensional) core dynamics model developed at NASA Goddard Space Flight Center. Our simulations focus on: (1) subcritical dynamos near the end of the Martian dynamo era; (2) the effects of Martian interior structures on the subcritical dynamo states; and (3) the geophysical implications of the subcritical dynamos on Martian magnetic anomalies and the evolution of Mars.

Our research objective is to answer fundamental science questions related to the observed magnetic anomaly: How much energy was needed to sustain the Martian dynamo? When and how was it terminated? What information or constraint could Martian magnetism provide to the evolution of Mars?

Relevance of Work to NASA: By studying Mars' magnetic properties, the research will improve knowledge of the planet's interior and its evolution history. It may identify geophysical mechanisms for the termination of the Martian dynamo, provide better interpretation of past observations and current missions to Mars, and potentially support scientific goals for future missions. It directly addresses NASA Planetary Science Research Objective 3C.1, "Learn how the Sun's family of planets and minor bodies originated and evolved," of the NASA Strategic Sub-Goal 3C, "Advance scientific knowledge of the origin and history of the solar system, the potential for life elsewhere, and the hazards and resources." It also contributes to Research Objectives 3C.2 and 3C.3 via investigation of Mars magnetic field evolution. Funding for this research comes through the NASA Mars Fundamental Research Program and the NASA Earth Surface and Interior Program.

Computational Approach: Our *m*MoSST core dynamics model uses a hybrid, spectral/finite-difference algorithm to solve a chaotic magnetohydrodynamic system in a rapidly rotating spherical shell. The code is written in Fortran 90/95 with modular structures. MPI libraries perform communication among distributed processors. We carry out most of our simulation runs with 128 processors for grid sizes up to 128×128×128. More resources are required for higher-resolution simulations.

Results: The research has shown, first, that the Martian dynamo can be subcritical, i.e., that the energy to sustain the dynamo can be lower than the critical energy necessary to excite the dynamo. Also, a subcritical dynamo tends to reverse more frequently than supercritical dynamos, resulting in a mean dipole field aligning closer to the equator (Figure 1). Furthermore, existence of a subcritical dynamo is not affected by the dimension of the inner core, though smaller inner cores would lead to smaller subcritical domains. Finally, a subcritical Martian dynamo could be terminated very quickly over a short period (fewer than 1 million years) by a small perturbation (e.g., less than 1% perturbation to the heat flow across the core-mantle boundary), and once terminated, it could not be reactivated even if the core's original geophysical state were restored.

Role of High-End Computing: We run all of our simulations on the NASA Advanced Supercomputing (NAS) facility's Columbia supercomputer. This system provides over 1 million processor-hours each year for our project, and we could not achieve our project goals without it. For example, simulations of subcritical dynamos require model domains at least of the order 100×100×100 for accurate determination of the critical points for onset and termination of the dynamo. A single simulation run needs approximately 100 processors for 240 wall-clock hours. The massive storage system at NAS is also necessary for archiving all numerical solutions (on the order of terabytes) for post-simulation analysis and other geophysical applications.

Future: Recent results from several research groups (including ours) suggest that the Martian dynamo might have been terminated in the Later Heavy Bombardment (LHB) period, which occurred between 3.8 and 4.1 billion years ago. The giant impacts during LHB could have provided sufficient perturbation to shut down a subcritical Martian dynamo. To further investigate this scenario, one must understand the properties of Martian dynamos in a heterogeneous thermodynamic environment resulting from giant impacts on Mars. This will be a focus for our future simulations. Another research activity will be geomagnetic data assimilation, in which we will use surface geomagnetic observations and our numerical geodynamo model to better understand the dynamics inside the Earth's core and its impact on changes of the Earth over long periods.

Co-Investigators

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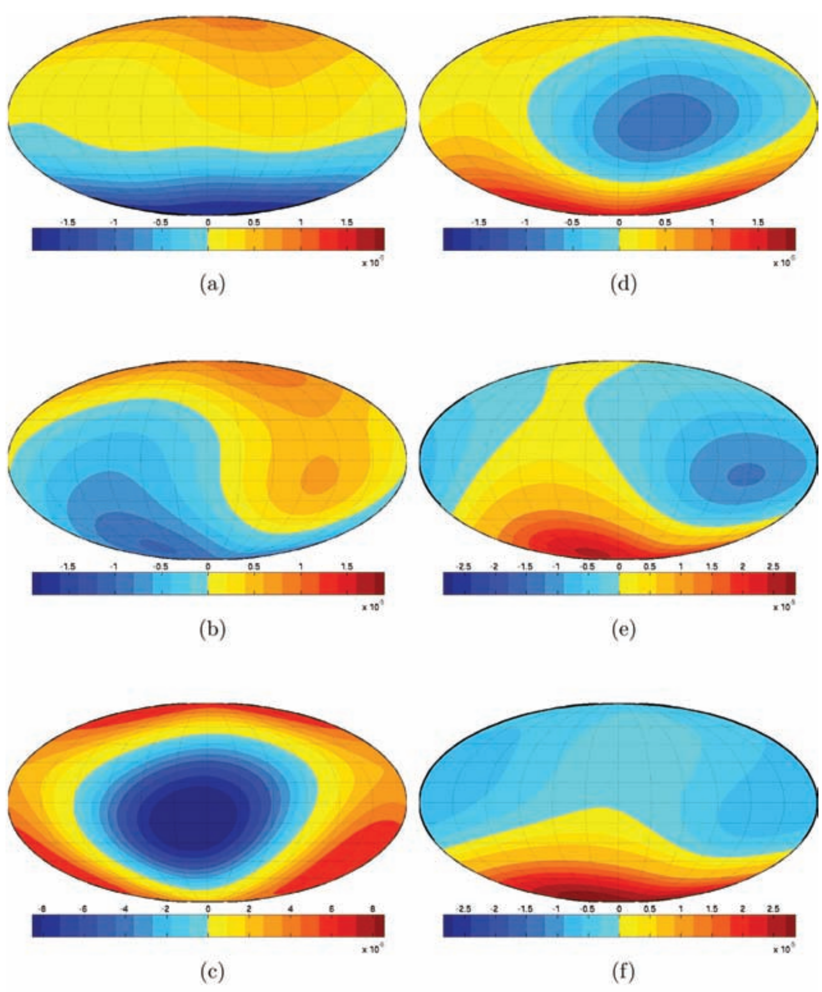
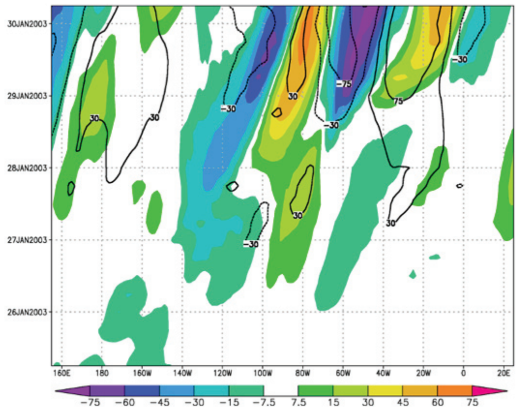


Figure 1: Snapshots of the radial component of the magnetic field at the surface of Mars during a reversal process. The polarity of the field in (a) reverses by the end of the process, shown in (f).

OBSERVING SYSTEM EXPERIMENTS: EVALUATING AND ENHANCING THE IMPACT OF SATELLITE OBSERVATIONS



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◀ **Figure 1:** Hovmoeller diagram (time upward) of the latitude-averaged (40N–80N) Advanced Infrared Spectrometer (AIRS)-induced impact on the 500 hectopascal (hPa) geopotential height between longitudes 160E and 20E. The shading represents the AIRS vs. Control difference (in meters). The solid lines represent the verifying National Centers for Environmental Prediction (NCEP) analyses minus the Control [1].

Project Description: This project aims to evaluate and optimize the use of satellite data, in particular the Advanced Infrared Spectrometer (AIRS), in global data assimilation and modeling. An Observing System Experiment (OSE) assesses the impact of an observational instrument by producing two or more data assimilation runs, one of which (the Control run) omits data from the instrument under study. From the resulting analyses, we initialize corresponding forecasts and evaluate them against the National Centers for Environmental Prediction (NCEP) operational analyses. A synoptic and dynamic evaluation then shows how the additional data propagate from the initial conditions and are amplified by the model's dynamics.

Relevance of Work to NASA: This work aims to improve modeling and prediction of weather and climate, and ultimately to increase our understanding of the Earth's atmosphere. Primary funding comes from NASA's Modeling, Analysis, and Prediction (MAP) Program. This work also contributes to a multi-agency team, the Joint Observing System Simulation Experiment (OSSE), led by M. Masutani at NCEP.

Computational Approach: The main tool for our work is the Goddard Earth Observing System Model, Version 5 (GEOS-5), provided by the Global Modeling and Assimilation Office (GMAO)—in particular its Data Assimilation System (DAS) and forecasting system. We also develop diagnostics to assess the impact of different instruments or datasets. We run the GEOS-5 DAS at a resolution of ½ degree longitude and latitude, with 72 vertical levels; forecasts have a resolution of ½ or ¼ degree.

Results: Our research has demonstrated the impact of quality-controlled AIRS observations under partly cloudy conditions. The improved coverage leads to a substantially different thermal structure in boreal winter conditions, particularly in the high latitudes. This improves forecast skill by enhancing the representation of the jet stream and baroclinic activity [1]. Figure 1 shows the impact of AIRS: between longitudes 120W and 20E, the AIRS 5-day forecast goes in the same direction as the NCEP analyses. This impact arises out of a substantially different representation of the mid-low tropospheric thermal structure in a data-poor region (northeastern Siberia and polar regions), which is captured in the AIRS analyses [1].

With the GMAO's L.P. Riishojgaard and E. Liu, we are also comparing the impact of AIRS temperature retrievals with that of clear-sky radiances. Despite an overall consensus that radiances are better, we have found that rejecting all data from cloud-contaminated areas, as done in the clear-sky radiance approach, severely reduces the spatial coverage and undermines the AIRS impact on the DAS and forecasting system.

In modeling tropical cyclogenetic processes, we have found that using AIRS data under partly cloudy conditions leads to better-defined tropical storms and improved GEOS-5 track forecasts. We performed two sets of experiments. One set centered on April–May 2008, when Tropical Cyclone Nargis hit Myanmar. The other centered on August–September 2006, overlapping with the NASA African Monsoon Multidisciplinary Analysis (NAMMA) observing campaign. The first of these studies aims to improve analysis and prediction of cyclones over the northern Indian Ocean. We are finding that AIRS strongly affects GEOS-5 analyses, leading to a deeper and better-located storm center. Clear-sky radiances have an intermediate impact, possibly due to less extensive coverage. As shown in Figure 2, AIRS temperature retrievals under partly cloudy conditions deepen Nargis' center, displaying a well-defined low and closed circulation not seen in the Control run. The corresponding forecasts compare well with the observed storm track.

In the second study, AIRS has improved the representation of African Easterly Waves, their interaction with Saharan air, and the organization of developing waves in closed circulations. We simulated the genesis of Hurricane Helene—observed at the end of the NAMMA campaign—using the GEOS-5 DAS with and without AIRS retrievals under partly cloudy conditions. The AIRS data significantly deepened the center of the simulated storm when the observed system was still an intensifying tropical storm. Forecasts initialized from these improved analyses led to more accurate storm tracks.

Finally, within the Joint OSSE team we contributed to assessing the suitability of the new Nature Run produced by the European Centre for Medium-Range Weather Forecasts (ECMWF) [2].

Role of High-End Computing: NASA High-End Computing (HEC) resources are crucial for this work. In the last 2 years, we have run about 70 month-long assimilation experiments at different resolutions and corresponding 5-day forecasts on the Explore supercomputer at the NASA Center for Computational Sciences and the Columbia supercomputer at the NASA Advanced Supercomputing facility. The mass storage allows us to continue analyzing model results with diagnostic tools that we have developed within the HEC environment.

Future: We are further investigating the impact of AIRS in the analysis and prediction of Tropical Cyclone Nargis. In collaboration with Riishojgaard and Liu, we are also comparing the retrieval and radiance approach from a global point of view, with rigorous and comprehensive tests in different conditions (boreal winter and boreal summer). We continue to study the impact of AIRS in modeling Atlantic cyclone development and the impact of model resolution on tropical cyclone representation, with forecasts at ½- and ¼-degree resolution.

In the future, we plan to assimilate retrievals of moisture, and temperature retrievals above clouds, for improved representation of the outflow above tropical cyclones. We will also evaluate the AIRS cloud-cleared radiances (that is, radiances that would be observed if the scene were clear), and will start assessing AIRS version 6 when available.

We will continue to benefit from collaboration with J. Susskind, Riishojgaard, and the GMAO, which provides GEOS-5 and frequent scientific and technical updates.

Co-Investigators

- William K. Lau, NASA Goddard Space Flight Center

Publications

[1] Reale, O., Susskind, J., Rosenberg, R., Brin, E., Liu, E., Riishojgaard, L.P., Terry, J., Jusem, J. C., "Improving Forecast Skill by Assimilation of Quality-Controlled AIRS Temperature Retrievals under Partially Cloudy Conditions," *Geophysical Research Letters*, Vol. 35, L08809, 2008.

[2] Reale, O., Terry, J., Masutani, M., Andersson, E., Riishojgaard, L.P., Jusem, J.C., "Preliminary Evaluation of the European Centre for Medium-Range Weather Forecasts (ECMWF) Nature Run over the Tropical Atlantic and African Monsoon Region," *Geophysical Research Letters*, Vol. 34, L22810, 2007.

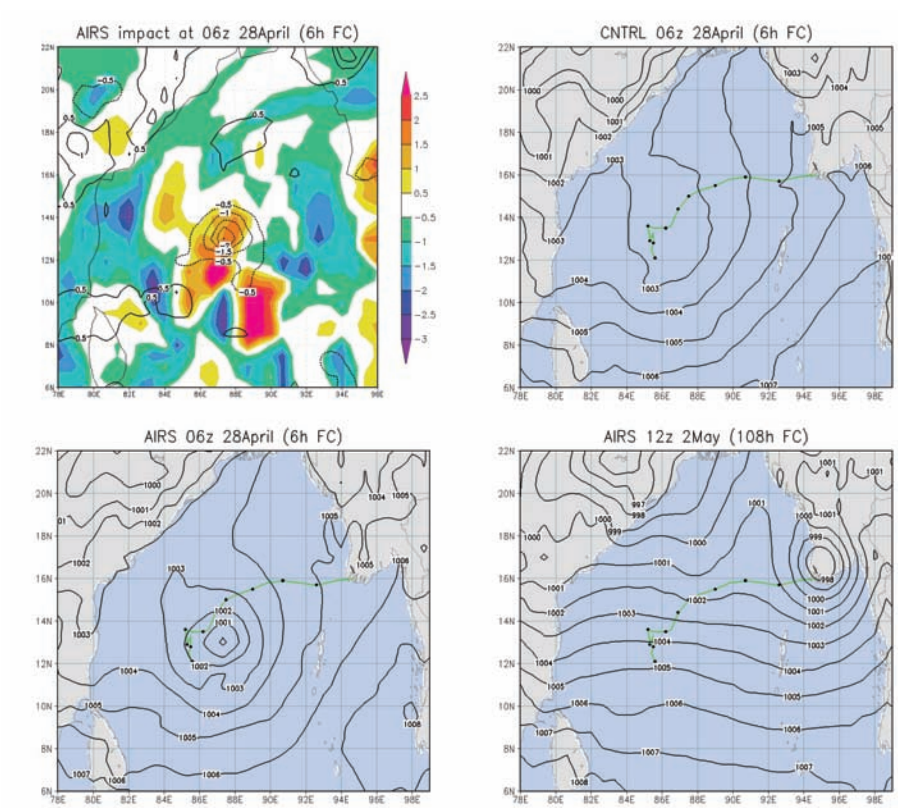
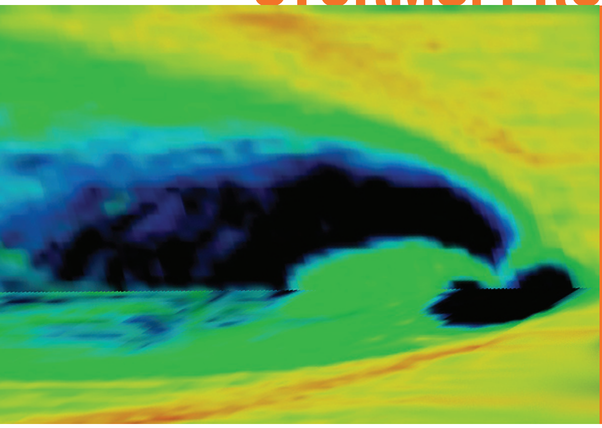


Figure 2: Impact of AIRS on the ½-degree Goddard Earth Observing System Model, Version 5 (GEOS-5) forecast for Tropical Cyclone Nargis. Upper left: Differences (AIRS minus Control) in 6-hour forecasts of 200 hPa temperature (°C, shaded) and sea-level pressure (hPa, solid line). Lower left: The 6-hour sea-level pressure forecast from the AIRS run shows a well-defined low close to the observed storm track (green solid line). Lower right: The corresponding 108-hour forecast for 2 May 2008 (landfall time) compares very well with the observed track. Upper right: The 6-hour sea-level pressure forecast from the Control run shows no detectable cyclone.

PLASMA REDISTRIBUTION DURING GEOSPACE STORMS: PROCESSES AND CONSEQUENCES



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◀ Close-up of Figure 2.

Project Description: This effort supports global modeling of the coupled solar wind, ionosphere, and magnetosphere through theoretical analysis and assimilation of observational results into empirical-statistical models. We are establishing: 1) how the flow of energy during geospace storms alters ionospheric plasma expansion into the magnetosphere and 2) how this expansion influences the dynamics and coupling of the solar wind, magnetosphere, and ionosphere to create these storms. Emphasis is on the inner magnetosphere's plasma and geomagnetic field conditions (including distortion by the ring current) and the evolution of ionospheric conductance, temperature, and densities. We aim to identify the principal features of plasma redistribution and to assess their impacts quantitatively over the range of storm conditions driven by the solar wind and the interplanetary magnetic field.

By comparing our model results with data from the Heliophysics Great Observatory, we validate the dynamic local response of source regions to solar wind influences and the simulated characteristics of the magnetospheric circulation. Resulting improvements in our simulation results lead toward enhanced global circulation models of geospace and its response to the dynamic heliosphere. We use data from the Advanced Composition Explorer (ACE), Wind, Geotail, and other missions to establish external drivers of the magnetospheric system. We also use data from Polar, the Fast Auroral SnapshoT (FAST), the Defense Meteorological Satellites Program (DMSP), and other low-Earth orbit missions to establish the spatial distribution and rate of ionospheric expansion; and data from the Polar, Imager for Magnetopause-to-Aurora Global Exploration (IMAGE), Cluster, and Department of Energy geosynchronous missions to make contact with observed magnetospheric responses.

Relevance of Work to NASA: Large-scale redistribution and restructuring of the ionosphere by storm-induced currents and electric fields produce massive ion plasma flows into the magnetosphere. Consequences include an enhanced polar wind, a heavy-ion auroral wind, and convective entrainment of the eroding plasmaspheric plumes. Entrained ionospheric plasmas populate the plasma sheet and ring current, modify magnetospheric convection and current systems, and thereby couple back into ionospheric plasma electrodynamics. We are taking major steps toward quantifying the effects of stormtime ionospheric restructuring on the magnetosphere and the dynamic development of this feedback—which are essential to forecasting near-Earth space weather. Funding for this research comes from NASA's Living With a Star Targeted Research and Development Program.

Computational Approach: This work uses a large number of theoretical and empirical models (Figure 1). We compute the outer magnetosphere and its interaction with the solar wind by integrating the equations of motion of millions of non-interacting charged particles in specified electric, magnetic, and gravitational fields. We make no drift approximations and integrate the full gyro-motion of the ions using adjustable resolution in space and time, based on a 4th-order Runge-Kutta scheme developed by collaborator Dominique Delcourt of the Centre d'Étude des Environnements Terrestre et Planétaires (CETP) in France.

We simulate the inner magnetosphere using the Comprehensive Ring Current Model (CRCM), which includes gyration and bounce-averaged particle motions, pitch-angle distributions, and charge exchange collisions. It also includes electrodynamic interaction with the ionosphere, leading to a self-consistent, stress-driven solution for the ring current pressure distribution. Outer magnetosphere results from the single-particle simulations supply the outer boundary condition.

Results: We successfully introduced the plasmasphere into the global circulation and outer magnetosphere configuration (Figure 2). We used the CRCM's plasmaspheric simulation to specify a source of cold ionospheric plasma at the outer boundary of the plasmasphere, where individual ions enter the outer magnetospheric circulation. The ions can return to the plasmasphere after substantial acceleration by the solar wind interaction, supplying energized ions back into the inner magnetosphere. We have implemented these capabilities using iterations of the outer and inner magnetospheric simulations [3].

Role of High-End Computing: Our primary computing platform is the Discover system at the NASA Center for Computational Sciences (NCCS). High-end computing is central to our work, owing to the large number of particle trajectories we need for bulk parameter calculations and kinetic work. To date, the particles are non-interacting, for simpler computation; yet the results have been well received and have motivated others in the global simulation community to develop multi-fluid codes that incorporate ionospheric plasmas as a dynamic element of the outer magnetosphere.

Future: Our next goal is to develop "virtual spacecraft" that can simulate the measurements of any particular spacecraft. This capability will facilitate comparing our results with specific spacecraft data. Having done this for fixed locations in space, our main work is to implement specified orbit parameters to enable the simulation to sample the magnetosphere as the spacecraft would do.

Another goal is to simulate particle trajectories using the new generation of global, multi-fluid simulations containing ionospheric plasma outflows in the circulation. Our first case will study only solar wind (ignoring ionospheric outflow) to test the multi-fluid code and prepare code interfaces for more interesting work that accounts for ionospheric outflows. This work will be of mainly technical interest, but it may lead to kinetic studies of solar wind ions.

Co-Investigators

- Mei-Ching H. Fok, NASA Goddard Space Flight Center

Publications

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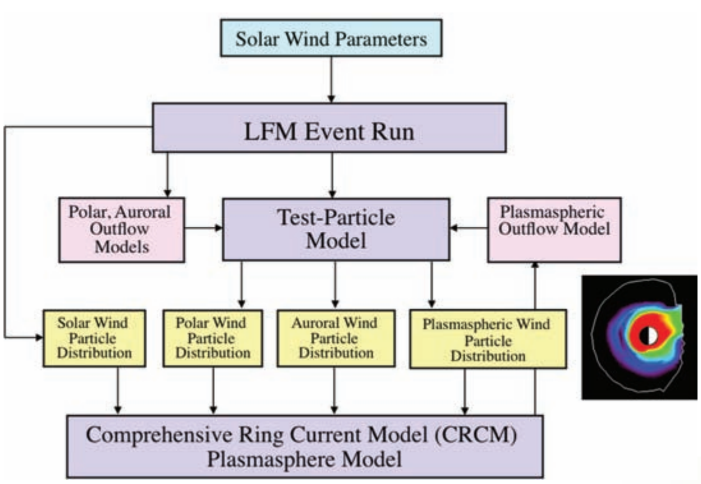


Figure 1: A simplified flowchart of a Global Ion Kinetic Model, which simulates plasma redistribution during solar storms. Solar wind parameters are inputs to the Lyon-Fedder-Mobarry (LFM) global fluid simulation, which computes the distribution of solar wind fluid in the magnetosphere. An empirical model specifies ionospheric outflows to generate test particle weightings and initial condition ranges and then launches millions of particles with random properties selected from those ranges. Resultant plasma properties serve as the boundary condition for the Comprehensive Ring Current Model (CRCM) of the inner magnetosphere. CRCM serves as a boundary condition for launching plasmaspheric ions back into the outer magnetosphere, where they circulate. These ions may return to the inner magnetosphere, where CRCM processes them.

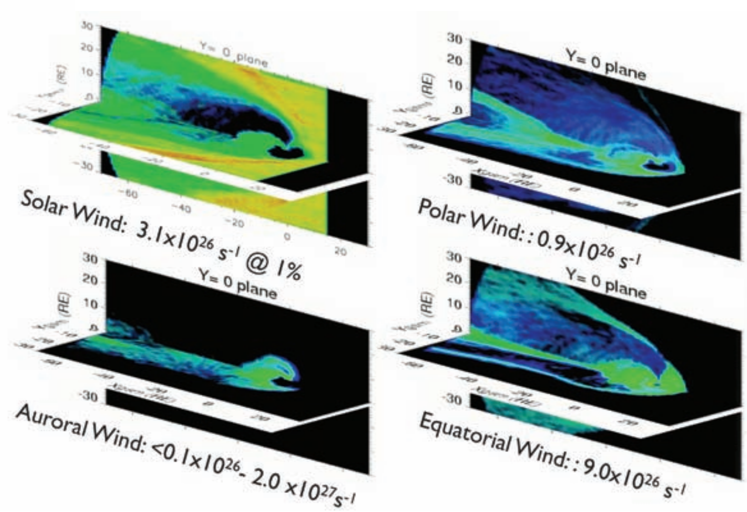
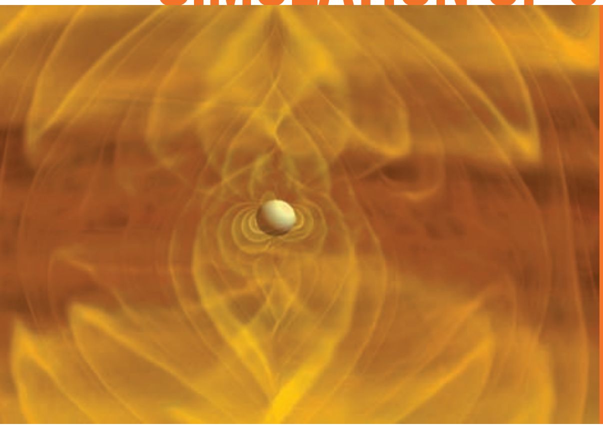


Figure 2: Distributions of multiple magnetospheric plasma populations as simulated using our global ion kinetic methods. Each case—Solar Wind, Polar Wind, Auroral Wind, and Equatorial (or Plasmaspheric) Wind—shows the density at a time representative of moderate magnetospheric convection flow in two planes. Labels under each plot indicate the fluence of ions into the magnetosphere.

SIMULATION OF COALESCING BLACK HOLE BINARIES



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◀ Detail of Figure 1.

Project Description: With support from NASA's Astrophysics Theory and Fundamental Astrophysics Program, we are simulating black hole binaries, in which black holes inspiral towards each other and merge into a single black hole remnant (Figure 1). Every stage of this process generates copious gravitational radiation; indeed, coalescing black holes are considered the most promising source of observable gravitational waves. Our simulations solve Einstein's field equations for spacetime using a finite-differencing code. The primary purpose of this work is to supply waveform templates for analyzing data from the planned Laser Interferometer Space Antenna (LISA) mission. Such templates are essential for performing matched filtering of the data and discerning signals from noise.

Relevance of Work to NASA: Understanding the dynamics and gravitational radiation of coalescing black holes is critical for the success of LISA and for meeting NASA science goals:

"Understand how the first stars and galaxies formed, and how they changed over time into the objects observed in the present universe": Calculating gravitational radiative recoil from asymmetric mergers helps to predict the probability that black holes will escape their host galaxies. By supplying waveform templates for LISA data analysis, we will aid both LISA and the ground-based Laser Interferometer Gravitational-Wave Observatory (LIGO) in pinpointing the positions and characteristics of the coalescing supermassive black holes that are believed to populate galactic cores, where they play central roles (literally) in galaxy evolution.

"Understand the origin and destiny of the universe, phenomena near black holes, and the nature of gravity": Black hole mergers may eventually serve as "standard candles," supplanting supernovae as the most accurate measure of the universe-expanding "dark energy." Accurately identifying and locating such mergers will require waveform templates for matched filtering of the data. Further, verification of our computed waveforms by laser interferometers will test Einstein's theory of general relativity to unprecedented precision and confirm the prediction of gravitational waves for the first time.

Computational Approach: We use a homegrown, finite-differencing code to solve Einstein's field equations. For adaptive mesh refinement (AMR) and parallelization, we currently use the PARAMESH software but are transitioning to an alternative AMR package called Carpet. Differencing and interpolation is currently 5th-order accurate. A 4th-order Runge-Kutta algorithm performs time-integration.

Results: We have made substantial scientific progress, including achievement of several milestones. We were the first to accurately compute the radiative recoil from an unequal mass binary and the first to simulate a merger preceded by as many as seven orbits. We have made important contributions to ongoing analytical efforts to model radiative recoil from binaries of arbitrary mass ratio and spins. We were the first to demonstrate consistency of numerical waveforms with post-Newtonian predictions. And we have contributed to waveform analysis in various other ways, including refinement of an effective-one-body, post-Newtonian model.

Our progress has benefited from significant technological developments. We developed coordinate conditions tailored to moving black holes and adapted these conditions for unequal mass binaries to facilitate sufficient numerical accuracy around the smaller black hole. Implementation of dissipation and constraint-damping has enabled stable and accurate evolutions of arbitrary duration. We have moved from a 2nd-order accurate to a fully 5th-order accurate evolution code and from 2nd-order to 6th-order accurate radiation extraction. We also have invented a novel algorithm for computing the spin of a black hole.

Role of High-End Computing: Our computational grid must have sufficient extent and resolution to simulate a vast region of physical space accurately, which includes the black hole sources, a "wave zone" where radiation is measured, and an outer boundary sufficiently removed to minimize reflections into the wave zone. Our simulations have often employed on the order of 10 million grid points, which have been just barely adequate so far—we desire an increase by at least an order of magnitude. At each grid point we store on the order of 100 double-precision variables. Consequently, running on a large number of parallel processors—at least 100 and ideally more than 1,000—is essential. Our calculations have benefited from such resources at both of NASA's High-End Computing Program facilities.

Future: First, we aim to simulate a mass ratio of greater than 10:1—which has never been done before—to verify analytic waveform models. Second we intend to simulate a variety of mass ratio and spin configurations, including exotic "transitional precession" events involving both large spin and mass ratio. Such exotic events may result in interesting exceptions to the relatively simple wave-forms simulated to date. Finally, we plan to model accretion disks around black holes, first with collisionless particles and then with a newly acquired hydrodynamic code. This research will determine whether electromagnetic correlates to gravitational radiation might be observable.

Co-Investigators

- John Baker, Joan Centrella, NASA Goddard Space Flight Center

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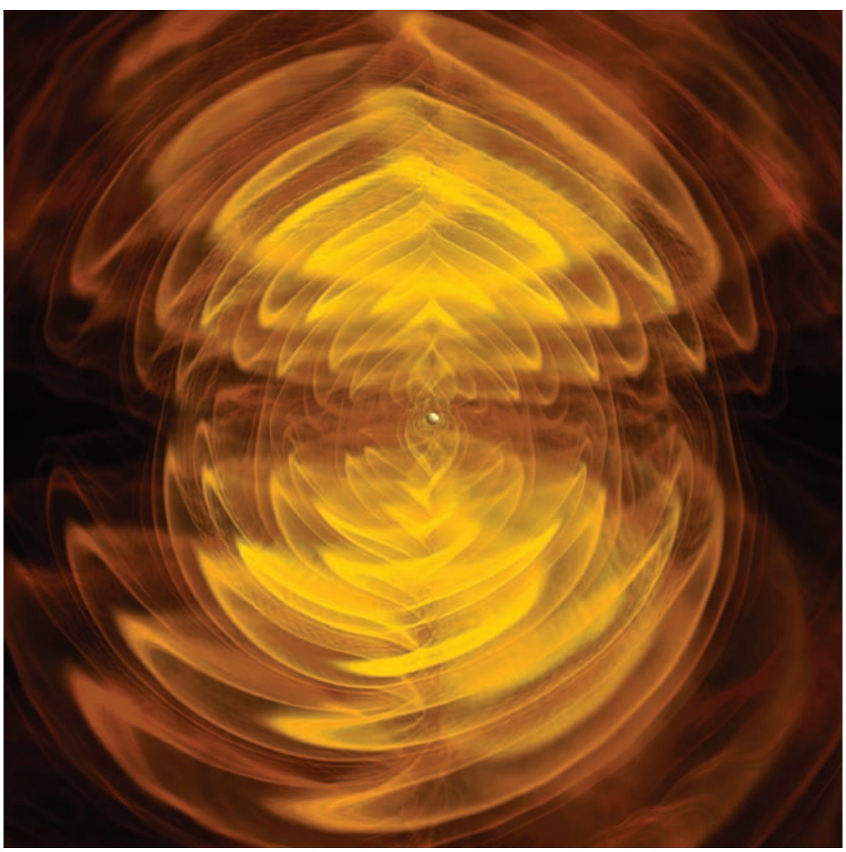

Figure 1: A simulation of X-polarized gravitational radiation from the merger of two black holes. The spherical shape in the center represents the horizon of the merged remnant. For a typical supermassive black hole of 1 million solar masses, this picture is on the order of 1 billion kilometers across.

SOLAR SURFACE MAGNETO-CONVECTION

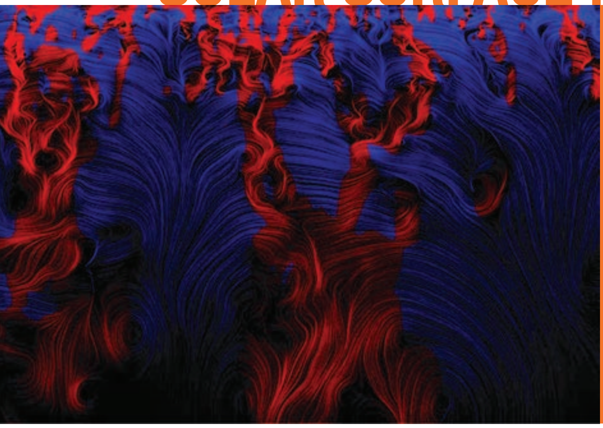

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Figure 1: Vertical cut through a 48-megameter (Mm)-wide simulation domain showing vertical velocity (red upward, blue downward) and streamlines near the solar surface (top of frame). Diverging upflows sweep downflows toward each other at the boundaries of the larger, deeper-lying upflows.

Project Description: The overall goal of this project is to understand the magneto-dynamics of the solar surface by making realistic simulations of surface magneto-convection and quantitatively comparing them with solar observations. The specific objectives are to investigate the nature of supergranulation and the evolution of the magnetic network; study the emergence of magnetic flux and its role in controlling the structure of the solar surface; and test and validate local helioseismology methods.

We perform simulations of: (i) supergranule-scale, quiet-Sun, solar-surface, hydrodynamic convection; (ii) supergranule-scale, quiet-Sun, solar-surface magneto-convection; (iii) very-high-resolution, granule-scale, solar-surface magneto-convection; and (iv) active-region evolution.

Relevance of Work to NASA: Funding for this research comes from NASA's Living With a Star (LWS) and Solar and Heliospheric Physics Programs. We use data from our simulations to interpret solar observations from the current Solar and Heliospheric Observatory (SOHO)/Michelson Doppler Imager and Hinode missions, and will do this in the future with the Solar Dynamics Observatory. We also use simulations to validate and improve observational analysis procedures, especially inversion methods in local helioseismology. Results from the magneto-convection simulations enhance our understanding of the solar magnetic field and our predictions of magnetic flux emergence before it is visible at the solar surface—an important goal of the LWS Program.

Computational Approach: Using a staggered 3D mesh, we solve the equations for mass, momentum, and internal energy in conservative form as well as the magnetic induction equation for fully compressible flow. The code uses finite differences, with 6th-order derivative operators and 5th-order interpolation operators. Time integration employs a 3rd-order, low-memory, Runge-Kutta scheme. We stabilize the code by diffusion in the momentum, energy, and induction equations. The grid is uniform in horizontal directions and non-uniform in the vertical (stratified) direction. Horizontal boundary conditions are periodic, while top and bottom boundary conditions are transmitting. By loading ghost zones at the top and bottom boundaries, we can use the same spatial derivative scheme throughout the domain.

We use a tabular equation of state, which includes local thermodynamic equilibrium (LTE) ionization of the abundant elements as well as hydrogen molecule formation, to obtain the pressure and temperature as a function of log density and internal energy per unit mass. We calculate the radiative heating/cooling by solving the radiation transfer equation in both continua and lines, assuming LTE. Using a multi-group method drastically reduces the number of wavelengths for which the transfer equation must be solved.

Results:

- *Simulation of supergranule-scale, hydrodynamic convection:* We study domains 48 and 96 megameters (Mm) wide and 20 Mm deep (Figures 1–3). The simulations cover only 10% of the geometric depth of the solar convection zone but 50% of its pressure-scale heights. They include all of the hydrogen and most of the helium ionization zones. The internal (ionization) energy flux is the largest contributor to the convective flux for temperatures less than 40,000 Kelvin; the thermal energy flux is the largest contributor at higher temperatures. The horizontal velocity spectrum is a power law, and the horizontal size of the dominant convective cells increases with depth. Convection arises from buoyancy work, which is largest close to the surface but significant over the entire domain. Two thirds of the area is upflowing fluid, except very close to the surface.
- *Application of simulation results to validate local helioseismic methods:* The simulations have a spectrum of resonant modes that agrees well (although sparser) with solar observations. We have performed time-distance and ring diagram analyses using the simulated photospheric velocities and have made comparisons with the simulation flowfield. We have found

that horizontal velocities can be determined down to several megameters below the surface, but vertical velocities cannot be accurately determined.

- *Magneto-convection simulations:* We have begun simulating both granule (6 Mm wide by 3 Mm deep) and supergranule scales (24 Mm wide by 20 Mm deep).

Role of High-End Computing: Without NASA's High-End Computing resources, we could not perform either the supergranule-scale or the high-resolution, granule-scale, magneto-convection simulations. We need to run the simulations for tens of thousands of time-steps on grids up to $1{,}000^2$ by 500. This project needs a large number of processors to obtain results in a reasonable amount of time. We get the greatest throughput with 125 processors on the Columbia system at the NASA Advanced Supercomputing (NAS) facility, although we could run efficiently with up to 1,000 processors. The NAS visualization group has been extremely helpful to us in interpreting our results.

Future: We intend to perform very-high-resolution (6 km horizontal and 5 to 14 km vertical), granule-scale (6 Mm wide by 3 Mm deep), magneto-convection simulations. They will have both initial vertical and horizontal field advected by inflows at the bottom into the computational domain. Supergranule-scale (48 Mm and 96 Mm wide by 20 Mm deep), magneto-convection simulations will have the initial horizontal field varying as a square root of density and horizontal flux advected into the domain by inflows at the bottom.

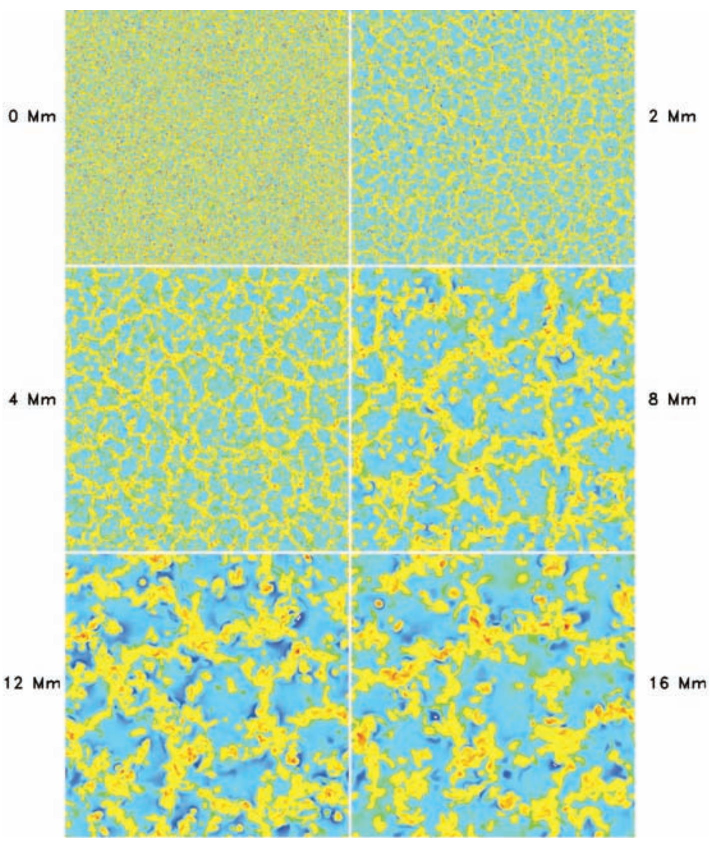

Figure 2: Horizontal slices at the solar surface (0) and 2, 4, 8, 12, and 16 Mm below the surface, showing vertical velocity. Red and yellow show downflows. Blue and green show upflows. The dominant horizontal scale of the convection increases monotonically with increasing depth.

Co-Investigators

- Åke Nordlund, Copenhagen University
- Dali Georgobiani, Werner Schaffenberger, Michigan State University
- David Benson, Kettering University

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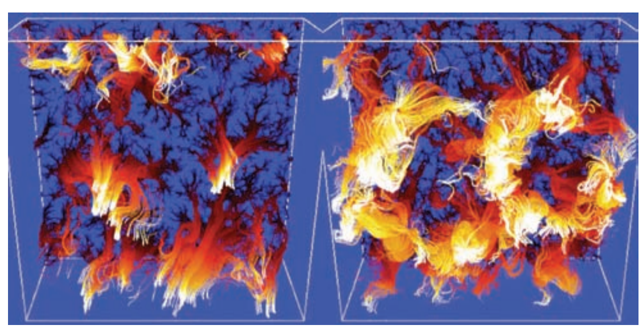

Figure 3: Fluid streamlines in a 48-Mm-wide simulation. In the left box, fluid moving up to the solar surface (background) originates from a small area in the upflow cells at the bottom (foreground). In the right box, fluid moving down from the surface (background) collects in the downflow boundaries of the large, supergranulation cells at the bottom (foreground).